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NBS MONOGRAPH 25—SECTION 5

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# Standard X-ray Diffraction Powder Patterns

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UNITED STATES DEPARTMENT OF COMMERCE
Alexander B. Trowbridge, *Secretary*
National Bureau of Standards • A. V. Astin, *Director*

# Standard X-ray Diffraction Powder Patterns

H. E. Swanson, H. F. McMurdie, M. C. Morris,
and E. H. Evans

National Bureau of Standards Monograph 25 — Section 5

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*Not previously listed in Powder Diffraction File.

**A mineral name in parentheses indicates a synthetic sample.

## Errata

### Monograph 25, Section 5

Circular 539

Vol. 1, p. 55; In the last column, the 7th entry should be I = 17, (for $d$ = 1.675).
Vol. 2, p. 28; The space group should be $T_h^7$-Ia3; the reference for it is:

> L. Pauling, and M. D. Shappell, The crystal structure of bixbyite and the C-modification of the sesquioxides, Z. Krist. **75**, 128-142 (1930).

Vol. 3, p. 27; The space group should be $T_h^7$-Ia3, from Pauling and Shappell, (ibid).
Vol. 3, p. 28; The space group should be $T_h^7$-Ia3, from Pauling and Shappell, (ibid).
Vol. 6, p. 12; The space group should be $D_{2h}^{16}$-Pmcn.
Vol. 8, p. 23; The line in the table reading: 503 1.5386 10 should follow the line: 610 1.5532 7.
Vol. 8, p. 25; The space group should be Ia3 (No. 206), from the reference:

> L. Pauling and M. D. Shappell, The crystal structure of bixbyite and the C-modification of the sesquioxides, Z. Krist. **75**, 128-142, (1930).

Monograph 25

Sec. 2, p. 23; The first two *hkl* entries for the pattern should be 002 and 102.

## STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Information on ten volumes in this series listed as follows is available from Mr. Howard E. Swanson, Room A221, Materials Building, National Bureau of Standards, Washington, D. C., 20234:

NBS Circular 539, Volume 1, Standard X-ray Diffraction Powder Patterns (Data for 54 substances).
NBS Circular 539, Volume 2, Standard X-ray Diffraction Powder Patterns (Data for 30 substances).
NBS Circular 539, Volume 3, Standard X-ray Diffraction Powder Patterns (Data for 34 substances).
NBS Circular 539, Volume 4, Standard X-ray Diffraction Powder Patterns (Data for 42 substances).
NBS Circular 539, Volume 5, Standard X-ray Diffraction Powder Patterns (Data for 45 substances).
NBS Circular 539, Volume 6, Standard X-ray Diffraction Powder Patterns (Data for 44 substances).
NBS Circular 539, Volume 7, Standard X-ray Diffraction Powder Patterns (Data for 53 substances).
NBS Circular 539, Volume 8, Standard X-ray Diffraction Powder Patterns (Data for 61 substances).
NBS Circular 539, Volume 9, Standard X-ray Diffraction Powder Patterns (Data for 43 substances).
NBS Circular 539, Volume 10, Standard X-ray Diffraction Powder Patterns (Data for 40 substances).

The following four volumes in this series are available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D. C., 20402, as follows:

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NBS Monograph 25, Section 2, Standard X-ray Diffraction Powder Patterns (Data for 37 substances) 35 cents.
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# STANDARD X-RAY DIFFRACTION POWDER PATTERNS

## Section 5.—Data for 80 substances

Howard E. Swanson, Howard F. McMurdie,[1] Marlene C. Morris,[1] and Eloise H. Evans[1]

Standard x-ray diffraction powder patterns are presented for 80 substances. Thirty-nine of these patterns represent experimental data and 41 are calculated. The experimental x-ray powder diffraction patterns are made with a Geiger counter x-ray diffractometer, using samples of high purity. All d-values were assigned Miller indices determined by comparison with theoretical interplanar spacings and from consideration of space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were obtained from published crystal structure data. The reported peak height intensities for calculated patterns were converted from integrated intensities.

Reference intensity values based upon the strongest line of corundum (113) in a 50 percent weight mixture are given for 73 materials.

Keywords: standard, x-ray diffraction, powder-patterns, crystal, structure, measurements, lattice, constants, reference-intensities

## INTRODUCTION

The X-ray Powder Diffraction File (1965)[2] is a compilation of diffraction patterns, gathered from many sources and produced under the auspices of the Joint Committee on Chemical Analysis by Powder Diffraction Methods.[3] The File is used for the identification of unknown crystalline materials by matching d-spacings and intensity measurements. Under the partial sponsorship of the Joint Committee, a program at the National Bureau of Standards contributes new data for this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents data for 80 compounds, 39 experimental and 41 calculated patterns. This compilation is the fifteenth of the series of "Standard X-ray Diffraction Powder Patterns."[4]

### Experimental Powder Patterns

**Powder Diffraction File Cards.** Under this heading are given the Powder Diffraction File card numbers and the literature reference for each card. Cards listed through the 1965 index to the Powder Diffraction File are included.

**Additional published patterns.** Literature references for patterns that have not been published as Powder Diffraction File cards are listed.

**NBS sample.** Many of the samples used to make NBS patterns were special preparations of high purity obtained from a variety of sources or prepared in small quantities in our laboratory. Treating the sample by appropriate annealing, recrystallizing, or heating in hydrothermal bombs improved the definition of most of the patterns.

Unless otherwise noted, the spectrographic analyses were done at NBS after preparation of the sample was completed. The limit of detection for the alkali elements was 0.05 percent for the spectrographic analyses. A check of phase purity was usually provided by the x-ray pattern itself, when it was indexed by comparison with theoretical d-values. A microscopic inspection for phase purity was also made on the nonopaque materials during the refractive index determination. The latter was done by grain-immersion methods in white light, with oils standardized in sodium light, in the range 1.40 to 2.1.

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts (1965).

**Structural data.** For cubic materials a value for the lattice constant was calculated for each d-value. However, the constant reported is that obtained by averaging the constants for the last five lines because of the greater accuracy of calculation in the high-angle region of the pattern. The unit cell values for noncubic substances were determined by means of a least-squares calculation made on the IBM 7094, using those d-values for which only one set of Miller indices could be assigned. The number of significant figures reported for the d-values in the NBS patterns varies slightly with the symmetry and crystallinity of each sample. The indexing and cell refinement calculation was performed using a program developed by Evans, Appleman, and Handwerker (1963). Lattice constant errors are given only for data refined on that program and are based on least-squares refinement of the variance-covariance matrix derived from the unweighted $\Delta\theta$ residuals.

---

[1] Research Associate at the National Bureau of Standards sponsored by the Joint Committee on Chemical Analysis by Powder Diffraction Methods.

[2] Dates in brackets indicate the literature references at the end of each section of this paper.

[3] This committee is composed of members from the American Society for Testing and Materials, the American Crystallographic Association, and the British Institute of Physics. Financial support is also provided by the National Bureau of Standards.

[4] See previous page for listing of other published volumes.

Published unit cell data in kX units and data given in angstrom units prior to 1947 were converted to angstrom units using the factor 1.00202 as recommended by an international conference of crystallographers reported in J. Sci. Instr. (1947).

The space groups are listed with both the Schoenflies and short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography (1952).

Orthorhombic cell dimensions are presented according to the Dana convention b>a>c (Dana System of Mineralogy, 1944).

The densities calculated from the NBS lattice constants are expressed in grams per cubic centimeter and are computed from the Avogadro number ($6.02252 \times 10^{23}$) and from atomic weights based on carbon 12 (Chem. Eng. News, 1961).

Intensity measurements. At least three patterns for intensity measurements were prepared to check reproducibility. Samples that gave satisfactory intensity patterns usually had an average particle-size smaller than 10 $\mu$ (Alexander et al., 1948). In order to avoid the orientation effects which occur when samples are packed or pressed, a sample holder was made that had an extended rectangular cavity opened on its top face and at one end. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see fig. 1). The powdered sample was then drifted into the end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample surface could be exposed to the x-ray beam (as shown in fig. 2). To powders that did not flow readily, or were prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the intensity of the strongest line.

Interplanar spacings. Specimens for the interplanar spacing patterns were prepared by packing into a shallow holder a sample containing approximately 5 wt. percent tungsten powder that served as an internal standard. When tungsten lines were found to interfere, 25 percent silver was used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used for the regions between the peaks of the standard. For low values of $2\theta$, the pattern peak was measured in the center, at a place averaging about 75 percent of the peak height. For higher values of $2\theta$, where $\alpha_1$ and $\alpha_2$ peaks were resolved, the $\alpha_1$ peak was measured in the same way. The internal standard correction appropriate to each region was then applied to the measurement of $2\theta$. The new internal standard lattice constants used were 3.16504 Å for tungsten and 4.08625 Å for silver at 25° C, as determined by Swanson, Morris, and Evans (1966). These changes increase d-values by a factor of 1.00004 when compared to the d-values obtained with the older standard samples. All of the NBS patterns, unless otherwise noted, are made on a diffractometer at 25° C using filtered copper radiation ($K\alpha_1$), having the wavelength 1.5405 Å. A curved lithium fluoride crystal monochromator was used in the preparation of some patterns.

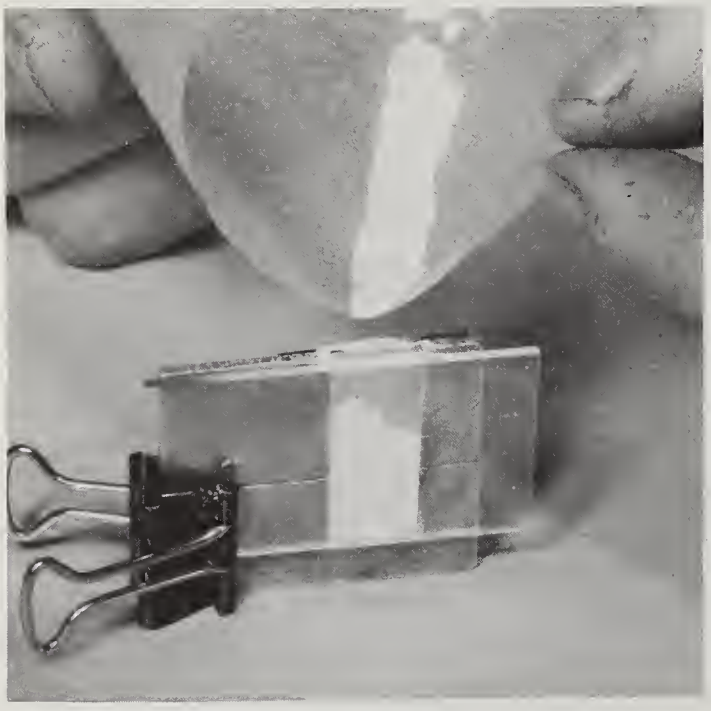

Figure 1

Figure 2

Since some substances are not readily available for experimental work, calculated powder patterns were made. These were based on published crystal structure data, using a FORTRAN program developed by Smith (1963).

Lorentz-polarization corrections are included. No corrections were made for temperature factors or absorption factors. Scattering factor values without ionization were taken from table 3.3.1A of the International Tables (1962a) for the following elements: beryllium, boron, calcium, cobalt, hydrogen, magnesium, nitrogen, oxygen, phosphorus, selenium, silver, and sulfur. All other scattering factor values used were taken from table 3.3.1B, International Tables (1962b).

Intensity calculations were based upon copper wavelength, 1.5405 Å. The integrated intensities printed out from the computer program were converted to peak height values by means of a graph from Swanson, Morris, Stinchfield, and Evans (1962). The peak height intensities are tabulated as percentages of the peak intensity of the strongest line. Peak height intensities from 0.1 to 0.9 were recorded as < 1; data with peak height intensities < 0.1 were omitted. When adjacent $2\theta$ values were nearly equal, resolution of individual peaks in the powder pattern would be unlikely. In that case, only one angle and its d-spacing are listed, with multiple *hkl's* and with the sum of the intensities of the peaks involved.

Literature references for calculated patterns are compiled at the end of that section.

The authors are indebted to J. H. deGroot for the preparation of many samples used, and to S. J. Carmel for his assistance on the work particularly in performing intensity measurements.

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Swanson, H. E., Morris, M. C., Stinchfield, R. P., and Evans, E. H. (1962). Standard X-ray Diffraction Powder Patterns, Natl. Bur. Std. U.S. Monograph 25, Sec. 1, 3.

The conversion factor for kX units to angstrom units (1947). J. Sci. Instr. **24**, 27.

The format of the first Powder Diffraction Cards issued by the Joint Committee had a space for a reference intensity in which NaCl was used. This original attempt to establish absolute values started by the Dow Chemical Co. however was not continued.

In 1961 de Wolff in Holland proposed that a variation of this idea be reconsidered as a help in evaluating mixtures. We expressed a desire to cooperate in the development of this project. After several reference materials were examined in both Delft and NBS labs, $\alpha Al_2O_3$ was chosen as an internal standard to be mixed 1:1 by weight. Corundum was picked partly because it is available commercially as Linde "A" in approximately one micron particle size from Union Carbide Corp., East Chicago, Ind., and partly because of its chemical stability and freedom from shape orientation in sample preparation.

The 1:1 mixture is mounted in our regular intensity sample holder (illust. p. 2) and it is necessary to run only the portion of the x-ray pattern that includes the strongest line of each compound; corundum (113), d= 2.085 Å was used. The direct ratio of the heights of the two lines is then reported as $I/I_{corundum}$. In a few instances the strongest line of one of the materials may fall on a line of the other. In this case the second strongest line is measured, and based upon previous knowledge of the relative peak heights, a correction is made thus enabling one to reconstruct the value for the strongest line.

In this report we are listing 35 $I/I_{corundum}$ values for some samples we have worked with in the past. Data reported from July 1965 has the $I/I_{corundum}$ value included in the text for each compound. We expect to continue measuring this value for new data submitted to the PDF.

## $I/I_{corundum}$ Values for Some Previously Reported Powder Patterns

| | |
|---|---|
| Aluminum 3:2 Silicate (mullite), $3Al_2O_3 \cdot 2SiO_2$ (orthorhombic) | 1.7 |
| Ammonium Fluoberyllate, $(NH_4)_2BeF_4$ (orthorhombic) | 0.6 |
| Ammonium Fluoborate, $NH_4BF_4$ (orthorhombic) | 0.7 |
| Barium Stannate, $BaSnO_3$ (cubic) | 6.1 |
| Bismuth Orthophosphate, $BiPO_4$ (monoclinic) | 4.7 |
| Bismuth Sulfide (bismuthinite), $Bi_2S_3$ (orthorhombic) | 2.1 |
| Cadmium Telluride, CdTe (cubic) | 6.5 |
| Calcium Fluoride Phosphate (fluorapatite), $Ca_5F(PO_4)_3$ (hexagonal) | 1.5 |
| Cesium Chromate, $Cs_2CrO_4$ (orthorhombic) | 1.4 |
| Cesium Fluoantimonate, $CsSbF_6$ (trigonal) | 2.7 |
| Cobalt Silicate, $Co_2SiO_4$ (orthorhombic) | 0.9 |
| Cobalt Tungstate, $CoWO_4$ (monoclinic) | 5.6 |
| Cobalt Titanate, $CoTiO_3$ (trigonal) | 1.5 |
| Erbium Arsenate, $ErAsO_4$ (tetragonal) | 3.1 |
| Europium(III) Vanadate, $EuVO_4$ (tetragonal) | 1.6 |

| | |
|---|---|
| Holmium Arsenate, $HoAsO_4$ (tetragonal) | 3.5 |
| Iridium Dioxide, $IrO_2$ (tetragonal) | 7.9 |
| Lead Boron Oxide, $PbB_4O_7$ (orthorhombic) | 2.5 |
| Lithium Phosphate, low form, (lithiophosphate), $Li_3PO_4$ (orthorhombic) | 1.1 |
| Lithium Phosphate, high form, $Li_3PO_4$ (orthorhombic) | 1.2 |
| Magnesium Ammonium Phosphate Hexahydrate (struvite), $MgNH_4PO_4.6H_2O$ (orthorhombic) | 1.0 |
| Neodymium Arsenate, $NdAsO_4$ (monoclinic) | 1.3 |
| Potassium Acid Phthalate, $C_6H_4$ (COOH) (COOK) (orthorhombic) | 1.4 |
| Potassium Zinc Decavanadate 16 Hydrate, $K_2Zn_2V_{10}O_{28}.16H_2O$ (triclinic) | 0.8 |
| Rubidium Chromate, $Rb_2CrO_4$ (orthorhombic) | 1.6 |
| Samarium Arsenate, $SmAsO_4$ (tetragonal) | 5.0 |
| Scandium Arsenate, $ScAsO_4$ (tetragonal) | 4.9 |
| Strontium Boron Oxide, $SrB_2O_4$ (orthorhombic) | 3.1 |
| Strontium Boron Oxide, $SrB_4O_7$ (orthorhombic) | 1.9 |
| Thallium Chromate, $Tl_2CrO_4$ (orthorhombic) | 3.0 |
| Tin Arsenide, SnAs (cubic) | 3.5 |
| Tin Fluoride, $SnF_2$ (monoclinic) | 2.7 |
| Titanium Dioxide, brookite, $TiO_2$ (orthorhombic) | 1.1 |
| Zinc Antimony Oxide, $ZnSb_2O_4$ (tetragonal) | 4.2 |
| Zinc Telluride, ZnTe (cubic) | 9.3 |

**Powder Diffraction File cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of ammonium cadmium chloride was precipitated at NBS from stoichiometric solutions of ammonium chloride and cadmium chloride.

Spectrographic analysis showed the major impurities to be less than 0.001 percent each of aluminum, barium, calcium, copper, magnesium, and silicon.

The sample was colorless and optically positive with a small 2V. $N_\alpha = 1.711$, $N_\beta = 1.714$, and $N_\gamma = 1.748$.

$I/I_{corundum} = 2.5$.

**Structural data.** Brasseur and Pauling (1938) determined that ammonium cadmium chloride has the space group $D_{2h}^{16}$-Pnam (No. 62) and $4(NH_4CdCl_3)$ per unit cell. Ammonium cadmium chloride is used as a structure type.

*Lattice constants*

| | *a*(Å) | *b*(Å) | *c*(Å) |
|---|---|---|---|
| Brasseur and Pauling (1938) | 8.98 | 14.90 | 3.98 |
| MacGillavry, et.al. (1939) | 9.02 | 14.93 | 3.97 |
| NBS, sample at 25°C | 9.017 | 14.911 | 3.9896 |

The density of ammonium cadmium chloride calculated from the NBS lattice constants is 2.932 g/cm$^3$ at 25° C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 7.71 | 89 | 110 | 11.47 |
| 7.44 | 100 | 020 | 11.87 |
| 5.745 | 65 | 120 | 15.41 |
| 4.509 | 15 | 200 | 19.67 |
| 4.348 | 5 | 130 | 20.41 |
| 4.316 | 6 | 210 | 20.56 |
| 3.857 | 10 | 220,011 | 23.04 |
| 3.728 | 4 | 040 | 23.85 |
| 3.541 | 43 | 111 | 25.13 |
| 3.445 | 17 | 140 | 25.84 |
| 3.340 | 27 | 230 | 26.67 |
| 3.110 | 5 | 031 | 28.68 |
| 2.987 | 30 | 201 | 29.89 |
| 2.945 | 8 | 310,131 | 30.32 |
| 2.930 | 36 | 211 | 30.48 |
| 2.873 | 15 | 240 | 31.10 |
| 2.833 | 15 | 150 | 31.55 |
| 2.787 | 12 | 320 | 32.08 |
| 2.773 | 58 | 221 | 32.25 |
| 2.608 | 2 | 141 | 34.35 |
| 2.573 | 10 | 330 | 34.84 |
| 2.487 | 10 | 250,060 | 36.09 |
| 2.396 | 25 | 160 | 37.51 |
| 2.340 | 2 | 340 | 38.44 |
| 2.285 | 16 | 321 | 39.40 |
| 2.255 | 1 | 400 | 39.95 |
| 2.158 | 6 | 420 | 41.83 |
| 2.117 | 3 | 350 | 42.68 |
| 2.111 | 6 | 251 | 42.80 |
| 2.073 | 4 | 170 | 43.62 |
| 2.053 | 14 | 161,430 | 44.07 |
| 2.018 | 24 | 341 | 44.87 |
| 1.994 | 11 | 002 | 45.45 |
| 1.963 | 4 | 401 | 46.21 |
| 1.929 | 9 | 440 | 47.07 |
| 1.927 | 9 | 022,270 | 47.12 |
| 1.915 | 1 | 360 | 47.44 |
| 1.9110 | 1 | 261 | 47.54 |
| 1.8978 | 13 | 421 | 47.89 |
| 1.8794 | 6 | 071 | 48.39 |
| 1.8642 | 2 | 080 | 48.81 |
| 1.8394 | 15 | 171 | 49.51 |
| 1.8253 | 7 | 431,180 | 49.92 |
| 1.7987 | 3 | 450 | 50.71 |
| 1.7533 | 2 | 520 | 52.12 |

## References

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MacGillavry, C.H., Nijveld, H., Dierdorp, S. and Karsten, J. (1939). Die Kristallstruktur von $NH_4CdCl_3$ und $RbCdCl_3$, Rec. trav. chim. **58**, 193-200.

| Internal standard W, a = 3.16504 Å<br>$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d* (Å) | *I* | *hkl* | 2θ(°) |
| 1.7384 | 4 | 370 | 52.60 |
| 1.7262 | 4 | 142,361 | 53.00 |
| 1.7229 | 4 | 280 | 53.11 |
| 1.7125 | 2 | 232 | 53.46 |
| 1.6952 | 1 | 530 | 54.05 |
| 1.6598 | 2 | 181 | 55.30 |
| 1.6394 | 3 | 451 | 56.05 |
| 1.6297 | 3 | 190 | 56.41 |
| 1.6236 | 3 | 540 | 56.64 |
| 1.5846 | 1 | 380 | 58.17 |
| 1.5811 | 3 | 281 | 58.31 |
| 1.5601 | 2 | 531 | 59.17 |
| 1.5562 | 4 | 252,062 | 59.33 |
| 1.5482 | 1 | 470 | 59.67 |
| 1.5436 | 1 | 550 | 59.87 |
| 1.5333 | 3 | 162 | 60.31 |
| 1.5084 | 3 | 191 | 61.41 |
| 1.5032 | 3 | 541,600 | 61.65 |
| 1.4735 | 3 | 620 | 63.03 |
| 1.4600 | 1 | 560 | 63.68 |
| 1.4515 | 4 | 352 | 64.10 |
| 1.4395 | 2 | 551 | 64.70 |
| 1.4371 | 3 | 172 | 64.82 |

Powder diffraction cards. None.

Additional published patterns. None.

NBS sample. The sample of ammonium manganese trifluoride was prepared at NBS by R.A. Forman from saturated solutions of ammonium fluoride and manganese chloride. The first 10 percent of the crystals were collected and washed in alcohol. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, calcium, iron, and magnesium.

The color of the sample was pinkish white. The index of refraction was 1.490.

$I/I_{corundum} = 3.2$.

Structural data. Simanov, Batsanova, and Kovba (1957) determined that ammonium manganese trifluoride has the perovskite structure, the space group $O_h^1$-Pm3m (No. 221) and 1 ($NH_4MnF_3$) per unit cell.

*Lattice constants*

| | *a*(Å) |
|---|---|
| Simanov, Batsanova, and Kovba (1957) | 4.239 |
| Hoppe, Liebe, and Dahne (1961) | 4.241 |
| NBS, sample at 25°C | 4.2410 |

The density of ammonium manganese trifluoride calculated from the NBS lattice constant is 2.829 g/cm³ at 25° C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) | *a* (Å) |
|---|---|---|---|---|
| 4.243 | 100 | 100 | 20.92 | 4.243 |
| 3.000 | 63 | 110 | 29.76 | 4.243 |
| 2.449 | 5 | 111 | 36.66 | 4.242 |
| 2.120 | 57 | 200 | 42.60 | 4.240 |
| 1.896 | 33 | 210 | 47.93 | 4.240 |
| 1.731 | 16 | 211 | 52.85 | 4.240 |
| 1.4994 | 18 | 220 | 61.82 | 4.241 |
| 1.4135 | 10 | 300 | 66.04 | 4.240 |
| 1.3414 | 5 | 310 | 70.09 | 4.242 |
| 1.2245 | 5 | 222 | 77.96 | 4.242 |
| 1.1763 | 3 | 320 | 81.81 | 4.241 |
| 1.1334 | 6 | 321 | 85.62 | 4.241 |
| 1.0605 | 3 | 400 | 93.16 | 4.242 |
| 1.0287 | 5 | 410 | 96.96 | 4.2414 |
| 0.9996 | 7 | 411 | 100.80 | 4.2409 |
| .9484 | 4 | 420 | 108.61 | 4.2414 |
| .9254 | 3 | 421 | 112.68 | 4.2407 |
| .9042 | 3 | 332 | 116.82 | 4.2411 |
| .8657 | 3 | 422 | 125.69 | 4.2410 |
| .8482 | 2 | 500 | 130.48 | 4.2410 |
| .8317 | 4 | 510 | 135.67 | 4.2409 |
| .8162 | 2 | 511 | 141.37 | 4.2411 |
| .7875 | 3 | 520 | 155.94 | 4.2408 |

## References

Hoppe, R., Liebe, W., and Dähne, W. (1961). Über Fluoromanganate der Alkalimetalle, Z. anorg. u. allgem. Chem. 307, 276-289.

Simanov, Yu. P., Batsanova, L.P., and Kovba, L.M. (1957). X-ray investigation of the binary fluorides of bivalent manganese, Russ. J. Inorg. Chem. 2, 207. (Translated from Zh. Neorgan. Khim. II, No. 10, 2410-2415).

Powder diffraction cards. None.

Additional published patterns. None

NBS sample. The sample of ammonium mercury trichloride was precipitated at NBS from solutions of ammonium chloride and mercury chloride.

Spectrographic analysis showed the only impurity greater than 0.001 percent to be 0.01 to 0.1 percent silicon.

The sample was light gray to colorless, and optically positive with the indices of refraction $N_o = 1.793$ and $N_e = 1.84$. The higher index could not be measured accurately because the liquid and sample reacted.

$I/I_{corundum} = 3.1$.

Structural data. Harmsen (1938) reported that ammonium mercury trichloride has one of several tetragonal space groups P*** and 1 ($NH_4HgCl_3$) per unit cell. Ammonium mercury trichloride is used as a structure type.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Harmsen (1938)---------- | 4.20 | 7.96 |
| NBS, sample at 25°C------ | 4.1977 ±0.0001 | 7.9353 ±0.0002 |

The density of ammonium mercury trichloride calculated from the NBS lattice constants is 3.859 g/cm³ at 25° C.

Reference

Harmsen, E.J. (1938). The crystal structure of $NH_4HgCl_3$, Z. Krist. **100A**, 208-211.

Internal standard Ag, a = 4.08625 Å
CuK$\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2$\theta$(°) |
|---|---|---|---|
| 7.93 | 100 | 001 | 11.15 |
| 4.200 | 56 | 100 | 21.14 |
| 3.967 | 23 | 002 | 22.39 |
| 3.711 | 38 | 101 | 23.96 |
| 2.969 | 44 | 110 | 30.07 |
| 2.883 | 47 | 102 | 30.99 |
| 2.782 | 22 | 111 | 32.15 |
| 2.645 | 18 | 003 | 33.86 |
| 2.377 | 33 | 112 | 37.81 |
| 2.239 | 18 | 103 | 40.25 |
| 2.099 | 13 | 200 | 43.06 |
| 2.029 | 9 | 201 | 44.62 |
| 1.983 | 18 | 004 | 45.71 |
| 1.974 | 17 | 113 | 45.93 |
| 1.877 | 8 | 210 | 48.45 |
| 1.855 | 6 | 202 | 49.06 |
| 1.827 | 13 | 211 | 49.88' |
| 1.793 | 10 | 104 | 50.88 |
| 1.6966 | 2 | 212 | 54.00 |
| 1.6491 | 11 | 114 | 55.69 |
| 1.6444 | 9 | 203 | 55.86 |
| 1.5868 | 2 | 005 | 58.08 |
| 1.5308 | 6 | 213 | 60.42 |
| 1.4843 | 3 | 105,220 | 62.52 |
| 1.4588 | 4 | 221 | 63.74 |
| 1.4417 | 4 | 204 | 64.59 |
| 1.3994 | 4 | 115,300 | 66.79 |
| 1.3899 | 5 | 222 | 67.31 |
| 1.3780 | 3 | 301 | 67.96 |
| 1.3635 | 4 | 214 | 68.79 |
| 1.3274 | 2 | 310 | 70.94 |
| 1.3227 | 2 | 006 | 71.23 |
| 1.3092 | 3 | 311 | 72.08 |
| 1.2943 | 5 | 223 | 73.04 |
| 1.2658 | 2 | 205 | 74.96 |
| 1.2616 | 4 | 106 | 75.25 |
| 1.2587 | 4 | 312 | 75.46 |
| 1.2366 | 2 | 303 | 77.05 |
| 1.2116 | 1 | 215 | 78.95 |
| 1.2081 | 2 | 116 | 79.22 |

| Internal standard Ag, a = 4.08625 Å<br>$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d* (Å) | *I* | *hkl* | 2θ(°) |
| 1.1881 | 4 | 224 | 80.83 |
| 1.1865 | 3 | 313 | 80.96 |
| 1.1646 | 2 | 320 | 82.81 |
| 1.1518 | 3 | 321 | 83.94 |
| 1.1434 | 2 | 304 | 84.70 |
| 1.1333 | 1 | 007 | 85.63 |
| 1.1190 | 2 | 206 | 87.00 |
| 1.1032 | 2 | 314 | 88.56 |
| 1.0944 | 2 | 107 | 89.47 |
| 1.0837 | 2 | 225 | 90.59 |
| 1.0810 | 2 | 216 | 90.88 |
| 1.0656 | 2 | 323 | 92.58 |
| 1.0590 | 2 | 117 | 93.33 |
| 1.0496 | 2 | 305,400 | 94.42 |
| 1.0184 | 3 | 315,410 | 98.29 |
| 1.0095 | 3 | 411 | 99.46 |
| 1.0043 | 2 | 324 | 100.16 |
| 0.9975 | 2 | 207 | 101.10 |
| .9920 | 1 | 008 | 101.88 |
| .9893 | 2 | 330 | 102.26 |
| .9874 | 3 | 226 | 102.54 |
| .9756 | 3 | 403 | 104.28 |
| .9706 | 3 | 217 | 105.05 |
| .9655 | 3 | 108 | 105.84 |
| .9612 | 3 | 306 | 106.51 |
| .9502 | 1 | 413 | 108.32 |
| .9408 | 3 | 118 | 109.91 |

**Powder Diffraction File cards.** No. 2-0545, Wallmark and Westgren (1937).

**Additional published patterns.** None.

**NBS sample.** The sample of barium aluminum oxide was prepared at NBS from gamma alumina and barium carbonate. The mixture was heated at 1200°C for 1 and 1/2 hrs.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of calcium, silicon, and vanadium.

The sample was colorless and had very low double refraction. The average index of refraction was approximately 1.675.

$I/I_{corundum} = 4.4$.

**Structural data.** Wallmark and Westgren (1937) determined that barium aluminum oxide has the space group $D_6^6$-$P6_322$ (No. 182).

Arlett, White, and Robbins (1967) found a doubling of the *a* axis and $8(BaAl_2O_4)$ per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Wallmark and Westgren [1937] | 5.220 | 8.779 |
| Glasser and Dent Glasser [1963] | 5.228 | 8.756 |
| Do Dinh and Bertaut [1965] | 5.227 | 8.802 |
| Arlett et al. [1967] | 10.444 | 8.793 |
| NBS, sample at 25°C | 10.4470 ±.0001 | 8.7940 ±.0002 |

The density of barium aluminum oxide, calculated from the NBS lattice constants is 4.080 g/cm³ at 25°C.

**Additional published patterns.** Do Dinh and Bertaut (1965).

Internal standard Ag, a = 4.08625 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 4.525 | 45 | 200 | 19.60 |
| 4.001 | 6 | 002 | 20.16 |
| 4.022 | 10 | 201 | 22.08 |
| 3.153 | 100 | 202 | 28.28 |
| 2.611 | 40 | 220 | 34.31 |
| 2.505 | 3 | 221 | 35.81 |
| 2.461 | 2 | 203 | 36.48 |
| 2.413 | <1 | 311 | 37.23 |
| 2.262 | 11 | 400 | 39.81 |
| 2.246 | 25 | 222 | 40.11 |
| 2.199 | 10 | 004 | 41.01 |
| 2.136 | <1 | 104 | 42.28 |
| 2.0111 | 19 | 402 | 45.04 |
| 1.9774 | 12 | 204 | 45.85 |
| 1.9505 | <1 | 223 | 46.52 |
| 1.7911 | <1 | 403 | 50.94 |
| 1.7098 | 5 | 420 | 53.55 |
| 1.6822 | 10 | 224 | 54.50 |
| 1.6391 | 1 | 205 | 56.06 |
| 1.5935 | 18 | 422 | 57.81 |
| 1.5764 | 7 | 404 | 58.50 |
| 1.5078 | 8 | 600 | 61.44 |
| 1.4771 | <1 | 423 | 62.86 |
| 1.4660 | 1 | 431,006 | 63.39 |
| 1.4263 | 1 | 602 | 65.37 |
| 1.3944 | 3 | 206 | 67.06 |
| 1.3890 | 1 | 405 | 67.36 |
| 1.3628 | <1 | 611 | 68.83 |
| 1.3496 | 6 | 424 | 69.60 |
| 1.3057 | 3 | 440 | 72.30 |
| 1.2782 | 5 | 531,226 | 74.11 |
| 1.2547 | 1 | 620 | 75.74 |
| 1.2516 | 2 | 442 | 75.96 |
| 1.2435 | 4 | 604 | 76.55 |
| 1.2299 | 1 | 406 | 77.55 |
| 1.2262 | 1 | 425 | 77.83 |
| 1.2063 | 6 | 622 | 79.36 |
| 1.1536 | <1 | 623 | 83.78 |
| 1.1308 | <1 | 800,631 | 85.87 |
| 1.1228 | 2 | 444 | 86.63 |
| 1.1129 | 2 | 426 | 87.59 |
| 1.0952 | 2 | 802 | 89.38 |
| 1.0898 | 2 | 624 | 89.95 |
| 1.0683 | 2 | 208 | 92.27 |
| 1.0549 | <1 | 803 | 93.80 |

| Internal standard Ag, a = 4.08625 Å<br>$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d* (Å) | *I* | *hkl* | 2θ(°) |
| 1.0511 | 1 | 811,606 | 94.24 |
| 1.0379 | 1 | 640 | 95.83 |
| 1.0216 | <1 | 625 | 97.87 |
| 1.0132 | <1 | 228 | 98.97 |
| 1.0100 | 2 | 642 | 99.39 |
| 1.0056 | <1 | 804 | 99.98 |
| 0.9885 | 1 | 408 | 102.38 |
| .9872 | 2 | 820 | 102.57 |
| .9783 | <1 | 643 | 103.87 |
| .9750 | 1 | 446 | 104.37 |
| .9632 | 1 | 822 | 106.20 |
| .9532 | 1 | 626 | 107.82 |
| .9431 | <1 | 911 | 109.52 |
| .9386 | 1 | 644 | 110.30 |
| .9247 | 2 | 428 | 112.81 |
| .9048 | <1 | 10.0.0 | 116.71 |
| .9005 | 1 | 824 | 117.59 |
| .8953 | <1 | 806 | 118.71 |
| .8938 | <1 | 645 | 119.04 |
| .8883 | <1 | 608 | 120.25 |
| .8861 | 1 | 10.0.2 | 120.74 |
| .8794 | <1 | 0.0.10 | 122.29 |
| .8728 | <1 | 905 | 123.89 |
| .8706 | 1 | 660 | 124.43 |
| .8632 | <1 | 2.0.10 | 126.33 |
| .8547 | <1 | 10.1.1 | 128.63 |
| .8470 | 1 | 646 | 130.85 |
| .8410 | <1 | 448 | 132.66 |
| .8391 | 2 | 842 | 133.25 |
| .8367 | 1 | 10.0.4 | 134.03 |
| .8334 | 1 | 2.2.10 | 135.11 |
| .8268 | 2 | 628 | 137.36 |
| .8188 | 2 | 826 | 140.34 |
| .8125 | <1 | 10.2.0 | 142.90 |
| .8094 | 1 | 664 | 144.19 |
| .7989 | 2 | 10.2.2 | 149.21 |
| .7968 | 2 | 844 | 150.35 |
| .7882 | <1 | 808 | 155.50 |

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Hoppe, R. and Schepers, B. (1960). Crystal structure of $BaGa_2O_4$ and $BaAl_2O_4$, Naturwissenschaften **47**, 376.

Wallmark, S. and Westgren, A. (1937). X-ray analysis of barium aluminates, Arkiv Kemi, Mineral. Geol. **B12**, No. 35.

**Powder Diffraction File cards.** No. 6-0333, National Bureau of Standards (1955). The following data is essentially the same as that reported on the above card: however, A. Glatz, Carrier Research and Development Co. suggested that if the pattern were remeasured, using his sample, it would be interesting to see the effect of back reflection lines on the lattice constants. The sharper pattern produced by this new sample also added weak front reflection lines.

**Additional published patterns.** None.

**NBS sample.** The high purity sample of bismuth sulfide, furnished by A. C. Glatz, was prepared by the method described in a paper by Glatz and Meikleham (1963). In addition, he also ground, sieved to -50 mesh, and annealed this sample at 400°C for one month.

The sample was a dark gray opaque powder.

$I/I_{corundum} = 2.1$.

**Structural data.** Hofmann (1933) determined that bismuth sulfide has the antimony sulfide structure, the space group $D_{2h}^{16}$-Pbnm (No. 62) and $4(Bi_2S_3)$ per unit cell.

*Lattice constants*

| | *a*(Å) | *b*(Å) | *c*(Å) |
|---|---|---|---|
| NBS (1955), sample at 26°C | 11.150 | 11.300 | 3.981 |
| NBS, sample at 25°C | 11.149 | 11.304 | 3.981 |

The density of bismuth sulfide calculated from NBS (1965) lattice constants is 6.806 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 7.936 | 1 | 110 | 11.14 |
| 5.654 | 22 | 020 | 15.66 |
| 5.566 | 6 | 200 | 15.91 |
| 5.040 | 22 | 120 | 17.58 |
| 3.967 | 42 | 220 | 22.39 |
| 3.748 | 17 | 101 | 23.72 |
| 3.569 | 100 | 130 | 24.93 |
| 3.530 | 58 | 310 | 25.21 |
| 3.253 | 16 | 021 | 27.39 |
| 3.118 | 80 | 230,211 | 28.60 |
| 2.824 | 14 | 040 | 31.65 |
| 2.812 | 51 | 221 | 31.80 |
| 2.717 | 28 | 301 | 32.94 |
| 2.709 | 4 | 410 | 33.04 |
| 2.641 | 18 | 311 | 33.91 |
| 2.521 | 40 | 240 | 35.58 |
| 2.499 | 12 | 420 | 35.91 |
| 2.456 | 10 | 231 | 36.55 |
| 2.305 | 20 | 041 | 39.04 |
| 2.258 | 32 | 141 | 39.90 |
| 2.241 | 12 | 430 | 40.20 |
| 2.188 | 5 | 510 | 41.22 |
| 2.130 | 7 | 241 | 42.39 |
| 2.118 | 11 | 421 | 42.65 |
| 2.096 | 9 | 250 | 43.13 |
| 2.075 | 10 | 520 | 43.59 |
| 1.990 | 18 | 002 | 45.54 |
| 1.985 | 16 | 440 | 45.66 |
| 1.953 | 39 | 431 | 46.45 |
| 1.945 | 31 | 501 | 46.66 |
| 1.937 | 16 | 151 | 46.87 |
| 1.932 | 10 | 350 | 47.00 |
| 1.919 | 18 | 530 | 47.32 |
| 1.884 | 23 | 060 | 48.26 |
| 1.857 | 13 | 600,160 | 49.00 |
| 1.853 | 16 | 251 | 49.11 |
| 1.834 | 10 | 610 | 49.67 |
| 1.785 | 4 | 260 | 51.13 |
| 1.780 | 8 | 222 | 51.28 |
| 1.765 | 5 | 620 | 51.74 |
| 1.750 | 8 | 540 | 52.21 |
| 1.738 | 33 | 132 | 52.60 |
| 1.734 | 14 | 312 | 52.74 |
| 1.703 | 11 | 061 | 53.77 |
| 1.683 | 4 | 161 | 54.46 |
| 1.680 | 4 | 360 | 54.58 |
| 1.665 | 2 | 611 | 55.12 |
| 1.606 | 4 | 451 | 57.30 |
| 1.603 | 2 | 541 | 57.45 |
| 1.587 | 2 | 550 | 58.07 |

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Internal standard W, a = 3.16504 Å
CuK$\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 1.562 | 11 | 242 | 59.09 |
| 1.552 | 7 | 640 | 59.49 |
| 1.548 | 7 | 361 | 59.69 |
| 1.537 | 4 | 631 | 60.14 |
| 1.5328 | 7 | 720 | 60.33 |
| 1.4828 | 11 | 171 | 62.59 |
| 1.4809 | 17 | 370,152 | 62.68 |
| 1.4451 | 6 | 271 | 64.42 |
| 1.4431 | 6 | 252 | 64.52 |
| 1.4359 | 8 | 522 | 64.88 |
| 1.4306 | 12 | 721 | 65.15 |
| 1.4127 | 1 | 080 | 66.08 |
| 1.4052 | 4 | 442 | 66.48 |
| 1.4018 | 4 | 180 | 66.66 |
| 1.3974 | 6 | 470 | 66.90 |
| 1.3862 | 4 | 352 | 67.51 |
| 1.3830 | 4 | 810 | 67.69 |
| 1.3814 | 8 | 532 | 67.78 |
| 1.3682 | 5 | 062 | 68.52 |
| 1.3580 | 2 | 162 | 69.11 |
| 1.3534 | 11 | 820,561 | 69.38 |
| 1.3498 | 5 | 651 | 69.59 |
| 1.3225 | 6 | 660 | 71.24 |
| 1.3184 | 4 | 471 | 71.50 |
| 1.3145 | 4 | 542 | 71.74 |
| 1.3101 | 10 | 741 | 72.02 |
| 1.3062 | 5 | 811 | 72.27 |
| 1.2950 | 6 | 281 | 72.99 |
| 1.2828 | 4 | 213 | 73.81 |
| 1.2587 | 4 | 223 | 75.46 |
| 1.2554 | 3 | 661 | 75.69 |
| 1.2482 | 10 | 190 | 76.21 |
| 1.2425 | 2 | 571 | 76.62 |
| 1.2310 | 1 | 910 | 77.47 |
| 1.2250 | 3 | 290 | 77.92 |
| 1.2145 | 4 | 722 | 78.72 |
| 1.2014 | 5 | 481,043 | 79.75 |
| 1.1938 | 3 | 143,580 | 80.36 |
| 1.1909 | 3 | 191 | 80.60 |
| 1.1880 | 7 | 372 | 80.83 |
| 1.1861 | 3 | 850,333 | 80.99 |
| 1.1830 | 4 | 901 | 81.25 |
| 1.1766 | 2 | 930,911 | 81.78 |
| 1.1656 | 4 | 671 | 82.73 |
| 1.1449 | 3 | 490 | 84.56 |
| 1.1432 | 8 | 472,581 | 84.72 |
| 1.1406 | 6 | 433,802 | 84.95 |
| 1.1380 | 2 | 153 | 85.19 |
| 1.1246 | 2 | 680 | 86.46 |
| 1.1093 | 1 | 10·1·0 | 87.95 |

Internal standard W, a = 3.16504 Å
CuK$\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 1.1079 | 4 | 2·10·0 | 88.09 |
| 1.1006 | 5 | 382,491 | 88.83 |
| 1.0940 | 1 | 590,10·2·0 | 89.50 |
| 1.0875 | 5 | 0·10·1 | 90.19 |
| 1.0823 | 2 | 681 | 90.74 |
| 1.0794 | 2 | 163 | 91.06 |
| 1.0570 | 6 | 192,780 | 93.55 |
| 1.0548 | 2 | 10·2·1 | 93.81 |
| 1.0475 | 2 | 912,4·10·0 | 94.67 |
| 1.0436 | 2 | 292,3·10·1 | 95.14 |
| 1.0410 | 1 | 363 | 95.45 |
| 1.0374 | 2 | 10·4·0 | 95.89 |
| 1.0350 | 2 | 960 | 96.18 |
| 1.0324 | 4 | 10·3·1 | 96.50 |
| 1.0236 | 1 | 582 | 97.61 |
| 1.0213 | 5 | 781,392 | 97.91 |
| 1.0196 | 5 | 871,703 | 98.13 |
| 1.0131 | 3 | 932 | 98.98 |
| 1.0106 | 4 | 463,2,11.0 | 99.31 |
| 1.0082 | 5 | 273 | 99.63 |
| 1.0040 | 2 | 10·4·1 | 100.20 |
| 1.0016 | 3 | 961 | 100.53 |
| 0.9953 | 2 | 004 | 101.41 |
| .9926 | 5 | 492 | 101.79 |
| .9910 | 2 | 1·11·1 | 102.02 |
| .9862 | 2 | 790 | 102.71 |
| .9830 | 2 | 970 | 103.18 |
| .9823 | 1 | 0·10·2,11·0·1 | 103.28 |
| .9794 | 3 | 2·11·1 | 103.71 |
| .9767 | 3 | 124,862 | 104.12 |
| .9761 | 3 | 214 | 104.21 |
| .9695 | 2 | 10·5·1,10·1·2 | 105.21 |
| .9681 | 3 | 11·2·1,2·10·2 | 105.43 |
| .9612 | 6 | 3·11·1 | 106.51 |
| .9590 | 4 | 743,592 | 106.87 |
| .9542 | 3 | 971,11·4·0 | 107.65 |
| .9480 | 1 | 234 | 108.68 |
| .9420 | 1 | 10·3·2,0·12·0 | 109.70 |
| .9385 | 5 | 1·12·0,6·10·1 | 110.31 |
| .9369 | 3 | 663,4·11·1 | 110.60 |
| .9336 | 1 | 782 | 111.19 |
| .9314 | 3 | 573,980,+ | 111.58 |
| .9258 | 2 | 12·1·0,244 | 112.60 |
| .9250 | 2 | 11·5·0 | 112.75 |
| .9184 | 1 | 962 | 114.00 |
| .9168 | 4 | 12·2·0 | 114.31 |
| .9011 | 4 | 11·5·1,2·11·2 | 117.48 |
| .8995 | 5 | 5·10·2 | 117.81 |
| .8982 | 5 | 7·10·1 | 118.09 |
| .8933 | 2 | 10·5·2,12·2·1 | 119.14 |

| Internal standard W, a = 3.16504 Å<br>CuK$\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d* (Å) | *I* | *hkl* | 2$\theta$(°) |
| 0.8865 | 1 | 3·11·2 | 120.37 |
| .8845 | 2 | 354,853 | 121.10 |
| .8826 | 3 | 12·4·0 | 121.56 |
| .8800 | 1 | 064,12·3·1 | 122.16 |
| .8774 | 1 | 8·10·0,604,+ | 122.78 |
| .8710 | 1 | 11·6·1 | 124.33 |
| .8678 | 2 | 4·11·2,520 | 125.13 |
| .8670 | 4 | 624,493 | 125.35 |
| .8605 | 3 | 11·4·2,0·10·3 | 127.04 |
| .8583 | 3 | 11·7·0 | 127.64 |
| .8575 | 3 | 1·10·3,8·10·1 | 127.87 |
| .8515 | 1 | 10·1·3,0·12·2 | 129.52 |
| .8490 | 1 | 1·12·2 | 130.24 |
| .8480 | 3 | 13·2·0 | 130.56 |
| .8471 | 4 | 1·13·1 | 130.80 |
| .8420 | 1 | 12·0·2 | 132.34 |
| .8417 | 1 | 714,2·12·2 | 132.44 |
| .8402 | 1 | 12·5·1 | 132.92 |
| .8398 | 2 | 6·12·0,12·1·2 | 133.02 |
| .8384 | 3 | 13·0·1 | 133.45 |
| .8364 | 2 | 7·10·2,13·3·0 | 134.11 |
| .8350 | 3 | 9·10·0 | 134.57 |
| .8337 | 2 | 10·9·0 | 134.99 |
| .8327 | 2 | 12·2·2,10·3·3 | 135.35 |
| .8303 | 5 | 4·13·0 | 136.16 |
| .8294 | 5 | 3·12·2,13·2·1 | 136.46 |
| .8281 | 2 | 3·13·1 | 136.92 |
| .8273 | 4 | 8·11·0 | 137.21 |
| .8260 | 3 | 374,873 | 137.64 |
| .8222 | 2 | 4·10·3 | 139.03 |
| .8200 | 2 | 6·11·2 | 140.01 |
| .8162 | 4 | 963,10·9·1 | 141.36 |
| .8127 | 2 | 4·13·1 | 142.79 |
| .8105 | 3 | 7·12·0,474 | 143.72 |
| .8070 | 3 | 0·14·0,12·4·2 | 145.30 |
| .8054 | 3 | 11·0·3,12·7·0 | 146.01 |
| .8035 | 2 | 11·1·3,8·10·2,+ | 146.94 |
| .7964 | 2 | 14·0·0 | 150.55 |
| .7955 | 3 | 664,5·12·2 | 151.07 |
| .7939 | 5 | 105,10·10·0 | 151.97 |
| .7893 | 2 | 973,12·7·1 | 154.74 |
| .7890 | 1 | 1·14·1,12·5·2 | 154.98 |
| .7884 | 2 | 14·2·0,2·13·2,+ | 155.37 |
| .7864 | 3 | 125,215 | 156.70 |
| .7836 | 3 | 2·14·1 | 158.82 |
| .7802 | 2 | 8·12·0,13·2·2 | 161.67 |

**Powder Diffraction File cards.** No. 2-1000, Holgersson (1930).

**Additional published patterns.** None.

**NBS sample.** The sample of cadmium chromite was prepared at NBS from cadmium oxide and chromium trioxide, dried before weighing, and heated in vacuum at 300°C for 17 hrs. The substance was ground, compressed into a pellet, and heated at 1050°C for 1 and 1/2 hrs.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of calcium and magnesium, and 0.001 to 0.01 percent each of aluminum, barium, copper, iron, manganese, nickel, antimony, and silicon.

The sample was gray olive green. The indices of refraction could not be determined because the sample was too fine-grained.

$I/I_{corundum} = 2.8$.

**Structural data.** Holgersson (1930) determined that cadmium chromite has the spinel structure with the space group $O_h^7$-Fd3m (No. 227) and 8($CdCr_2O_4$) per unit cell.

*Lattice constants*

| | *a*(Å) |
|---|---|
| Holgersson (1930) | 8.61 |
| Krause and Thiel (1934) | 8.59 |
| Verwey and Heilmann (1947) | 8.584 |
| NBS, sample at 25°C | 8.597 |

The density of cadmium chromite calculated from the NBS lattice constants is 5.862 g/cm$^3$ at 25°C.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 4.959 | 3 | 111 | 17.87 |
| 3.036 | 74 | 220 | 29.39 |
| 2.589 | 100 | 311 | 34.61 |
| 2.480 | 4 | 222 | 36.19 |
| 2.146 | 2 | 400 | 42.06 |
| 1.972 | 6 | 331 | 45.98 |
| 1.755 | 22 | 422 | 52.08 |
| 1.654 | 32 | 511 | 55.50 |
| 1.519 | 30 | 440 | 60.93 |
| 1.3592 | 7 | 620 | 69.04 |
| 1.3107 | 9 | 533 | 71.98 |
| 1.2956 | 2 | 622 | 72.95 |
| 1.1486 | 10 | 642 | 84.23 |
| 1.1188 | 12 | 731 | 87.02 |
| 1.0745 | 3 | 800 | 91.59 |
| 1.0131 | 4 | 822 | 98.98 |
| 0.9926 | 8 | 751 | 101.79 |
| .9164 | 3 | 664 | 114.38 |
| .9012 | 6 | 931 | 117.44 |
| .8775 | 8 | 844 | 122.75 |
| .8311 | 8 | 951 | 135.88 |

## References

Holgersson, S. (1930). Röntgenographische Untersuchungen einiger Synthetisch Dargestellten Chromspinelle, Z. anorg. u. allgem. Chem. 192, 123-128.

Krause, O. and Thiel, W. (1934). Über Keramische Farbkörper I, Ber. deut. keram. Ges. 15, 101-110.

Verwey, E. J. W. and Heilmann, E. L. (1947). Physical properties and cation arrangement of oxides with spinel structures, J. Chem. Phys. 15, 174-180.

**Powder Diffraction File cards.** No. 3-0860 (synthetic), Clark (1946) and No. 11-654 (natural), deWolff (1961).

**Additional published patterns.** Kuno and Hess (1953).

**NBS sample.** The sample of diopside was obtained from Tem-pres Research Inc., State College, Pa.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of aluminum, nickel, and strontium; and 0.01 to 0.1 percent each of iron, sodium, and titanium.

The sample was colorless and optically positive with indices of refraction $N_\alpha = 1.674$, $N_\beta = 1.680$, and $N_\gamma = 1.700$. 2V is medium.

$I/I_{corundum} = 1.0$.

**Structural data.** Wyckoff and Merwin (1925) determined that diopside has the space group $C_{2h}^6$-C2/c (No. 15) and 4 $[CaMg(SiO_3)_2]$ per unit cell.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 4.462 | 5 | 020 | 19.88 |
| 4.407 | 1 | $\bar{1}11$ | 20.13 |
| 3.660 | 3 | 111 | 24.30 |
| 3.343 | 11 | 021 | 26.64 |
| 3.231 | 28 | 220 | 27.58 |
| 2.992 | 100 | $\bar{2}21$ | 29.84 |
| 2.951 | 32 | 310 | 30.26 |
| 2.894 | 42 | $\bar{3}11$ | 30.87 |
| 2.838 | 3 | 130 | 31.50 |
| 2.566 | 25 | $\bar{1}31$ | 34.93 |
| 2.524 | 64 | 002 | 35.53 |
| 2.518 | | $\bar{1}12, 221$ | 35.63 |
| 2.389 | 3 | 131 | 37.61 |
| 2.301 | 16 | 311 | 39.12 |
| 2.215 | 13 | 112 | 40.70 |
| 2.198 | 13 | $\bar{2}22, 022$ | 41.02 |
| 2.156 | 12 | 330 | 41.87 |
| 2.133 | 18 | $\bar{3}31$ | 42.34 |
| 2.108 | 10 | $\bar{4}21$ | 42.86 |
| 2.075 | 1 | 420 | 43.57 |
| 2.042 | 19 | 041 | 44.33 |
| 2.014 | 14 | $240, \bar{4}02$ | 44.97 |
| 2.006 | 10 | 202 | 45.15 |
| 1.968 | 8 | $\bar{1}32$ | 46.07 |
| 1.860 | 3 | 331 | 48.93 |
| 1.835 | 9 | $510, \bar{4}22$ | 49.64 |
| 1.831 | | 222 | 49.76 |
| 1.813 | 3 | 132 | 50.29 |
| 1.774 | 2 | 421 | 51.46 |
| 1.754 | 13 | 150 | 52.10 |
| 1.720 | 2 | $\bar{5}12$ | 53.22 |
| 1.684 | 2 | $\bar{1}51$ | 54.45 |
| 1.673 | 6 | $042, \bar{2}42$ | 54.83 |
| 1.658 | 6 | $\bar{3}13$ | 55.37 |
| 1.624 | 33 | $\bar{5}31, \bar{2}23$ | 56.61 |
| 1.617 | | 440 | 56.90 |
| 1.586 | 1 | 530 | 58.11 |
| 1.562 | 3 | 600 | 59.08 |
| 1.550 | 5 | 350 | 59.59 |
| 1.529 | 3 | $\bar{6}02$ | 60.49 |
| 1.523 | 6 | 402 | 60.75 |
| 1.5096 | 2 | $\bar{5}32$ | 61.36 |
| 1.5034 | 11 | $\bar{1}33$ | 61.64 |
| 1.4918 | 2 | 242 | 62.17 |
| 1.4877 | 5 | 060 | 62.36 |
| 1.4750 | 1 | 620 | 62.96 |
| 1.4609 | 2 | 441 | 63.64 |
| 1.4469 | 3 | $\bar{6}22$ | 64.33 |
| 1.4267 | 8 | 061 | 65.35 |
| 1.4225 | 17 | 531 | 65.57 |

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Clark, C.B. (1946). X-ray diffraction data for compounds in the system CaO-MgO-$SiO_2$, J. Am. Ceram. Soc. 29, 25-30.

Futergendler, S.I. (1958). X-ray study of solid inclusions in diamonds, Soviet Phys.-Cryst. 3, 494.

Kuno, H. and Hess, H.H. (1953). Unit cell dimensions of clinoenstatite and pigeonite in relation to other common clinopyroxenes, Am. J. Sci. 251, 741-752.

Wyckoff, R.W.G. and Merwin, H.E. (1925). The space group of diopside $[CaMg(SiO_3)_2]$, Am. J. Sci. 9, 379-394.

| Internal standard W, a = 3.16504 Å<br>$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d* (Å) | *I* | *hkl* | 2θ(°) |
| 1.4086 | 10 | $\bar{3}52$ | 66.30 |
| 1.4072 | | 152 | 66.37 |
| 1.3895 | 3 | 223 | 67.33 |
| 1.3755 | 2 | $\bar{7}11$ | 68.11 |
| 1.3439 | 1 | 043 | 69.94 |
| 1.3305 | 7 | $\bar{7}12$ | 70.75 |
| 1.3269 | 7 | 621,512 | 70.97 |
| 1.3168 | 3 | $\bar{5}33$ | 71.60 |
| 1.2824 | 7 | $\bar{2}62$,062 | 73.83 |
| 1.2624 | 5 | $\bar{4}61$,004 | 75.20 |
| 1.2480 | 4 | 352 | 76.22 |
| 1.2362 | 2 | $\bar{1}71$ | 77.08 |
| 1.2222 | 1 | 532 | 78.13 |
| 1.2174 | 2 | $\bar{4}24$ | 78.50 |
| 1.2147 | 2 | 171,024 | 78.71 |

*Lattice constants*

| | *a*(Å) | *b*(Å) | *c*(Å) | β(°) |
|---|---|---|---|---|
| Wyckoff and Merwin (1925) | 9.73 | 8.91 | 5.25 | 105.83° |
| Kuno and Hess (1953) | 9.731 | 8.930 | 5.249 | 105.43° |
| Futergendler (1958) | 9.70 | 8.91 | 5.22 | 105° |
| deWolff (1961) | 9.761 | 8.926 | 5.258 | 105.79° |
| NBS, sample at 25°C | 9.748 | 8.926 | 5.250 | 105.86° |

The density of diopside calculated from the NBS lattice constants is 3.273 g/cm$^3$ at 25° C.

**Powder Diffraction File cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of cesium cadmium trichloride was made at NBS by fusing stoichiometric amounts of cesium chloride and cadmium chloride.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent sodium, and 0.01 to 0.1 percent each of barium, calcium, potassium, rubidium, and strontium.

The sample was colorless. It was optically positive with indices of refraction $N_o = 1.737$ and $N_e = 1.750$.

$I/I_{corundum} = 2.6$.

**Structural data.** Siegel and Gebert (1964) determined that cesium cadmium trichloride has the hexagonal barium titanate structure, the space group $D_{6h}^4$-$P6_3/mmc$ (No. 194) and 6($CsCdCl_3$) per unit cell. Ferrari and Baroni (1927) reported that there also exists a pseudocubic perovskite form of cesium cadmium trichloride.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Siegel and Gebert (1964) | 7.418 | 18.39 |
| NBS, sample at 25°C | 7.416 | 18.440 |

The density of cesium cadmium trichloride calculated from the NBS lattice constants is 3.989 g/cm$^3$ at 25°C.

Internal standard Ag, a = 4.08625 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 6.070 | 18 | 101 | 14.58 |
| 5.266 | 4 | 102 | 16.82 |
| 4.440 | 20 | 103 | 19.98 |
| 3.743 | 92 | 104 | 23.75 |
| 3.708 | 100 | 110 | 23.98 |
| 3.198 | 19 | 105 | 27.87 |
| 3.072 | 9 | 006 | 29.04 |
| 3.032 | 11 | 202 | 29.43 |
| 2.846 | 35 | 203 | 31.40 |
| 2.635 | 62 | 204 | 33.99 |
| 2.438 | 12 | 107 | 36.84 |
| 2.422 | 18 | 205 | 37.08 |
| 2.259 | 4 | 213 | 39.88 |
| 2.170 | 6 | 108 | 41.58 |
| 2.147 | 30 | 214 | 42.04 |
| 2.142 | 33 | 300 | 42.16 |
| 2.037 | 10 | 207 | 44.43 |
| 2.027 | 12 | 215 | 44.66 |
| 1.958 | 5 | 118 | 46.33 |
| 1.952 | 4 | 109 | 46.48 |
| 1.873 | 14 | 208 | 48.57 |
| 1.853 | 24 | 220 | 49.11 |
| 1.785 | 8 | 217 | 51.12 |
| 1.774 | 3 | 311 | 51.48 |
| 1.727 | 8 | 209 | 52.98 |
| 1.710 | 2 | 313 | 53.53 |
| 1.672 | 6 | 218 | 54.88 |
| 1.6614 | 8 | 314,307 | 55.24 |
| 1.6218 | 2 | 1·0·11 | 56.71 |
| 1.6034 | 4 | 315 | 57.42 |
| 1.5880 | 3 | 226 | 58.03 |
| 1.5652 | 4 | 219 | 58.96 |
| 1.5530 | 4 | 403 | 59.47 |
| 1.5370 | 4 | 0·0·12 | 60.15 |
| 1.5158 | 7 | 404 | 61.08 |
| 1.4752 | 5 | 317 | 62.95 |
| 1.4721 | 6 | 405 | 63.10 |
| 1.4324 | 2 | 323 | 65.06 |
| 1.4200 | 5 | 1·11·2 | 65.70 |
| 1.4095 | 3 | 318 | 66.25 |

## References

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Siegel, S. and Gebert, E. (1964). The structure of hexagonal $CsCdCl_3$ and tetragonal $Cs_2CdCl_4$, Acta Cryst. **17**, 790.

| Internal standard Ag, a = 4.08625 Å<br>$CuK_{\alpha_1}$ λ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d* (Å) | *I* | *hkl* | 2θ(°) |
| 1.4015 | 9 | 410 | 66.68 |
| 1.3794 | 3 | 2·1·11 | 67.89 |
| 1.3712 | 3 | 407 | 68.35 |
| 1.3679 | 3 | 325 | 68.54 |
| 1.3446 | 3 | 319 | 69.90 |
| 1.3410 | 2 | 414 | 70.11 |
| 1.3177 | 3 | 408 | 71.54 |
| 1.2860 | 1 | 327 | 73.59 |
| 1.2636 | 3 | 409 | 75.11 |
| 1.2482 | 6 | 3·0·12 | 76.21 |
| 1.2412 | 3 | 328 | 76.71 |
| 1.2373 | 4 | 504,417 | 77.00 |
| 1.2205 | 2 | 3·1·11 | 78.26 |
| 1.1961 | 3 | 329 | 80.18 |
| 1.1906 | 3 | 423 | 80.62 |
| 1.1830 | 6 | 2·2·12 | 81.25 |
| 1.1737 | 5 | 424 | 82.03 |
| 1.1528 | 4 | 425 | 83.85 |

**Powder Diffraction File cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of cesium calcium trichloride was prepared by fusing cesium chloride and anhydrous calcium chloride at approximately 900°C.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent strontium; and 0.01 to 0.1 percent each of potassium, sodium, and rubidium.

$I/I_{corundum} = 3.8$.

The sample was colorless. The index of refraction was 1.599.

**Structural data.** No structural information was found in the literature on cesium calcium trichloride; however it appears to be cubic and similar to other perovskites, with the space group $O_h^1$-Pm3m (No. 221) and 1 ($CsCaCl_3$) per unit cell.

This material gave x-ray patterns which showed no splitting and can be considered fully cubic at 25°C.

*Lattice constants*

| | *a*(Å) |
|---|---|
| NBS, sample at 25°C | 5.396 |

The density of cesium calcium trichloride calculated from the NBS lattice constant is 2.952 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 5.394 | 15 | 100 | 16.42 |
| 3.819 | 100 | 110 | 23.27 |
| 3.115 | 71 | 111 | 28.63 |
| 2.698 | 78 | 200 | 33.17 |
| 2.413 | 7 | 210 | 37.23 |
| 2.203 | 33 | 211 | 40.92 |
| 1.908 | 30 | 220 | 47.62 |
| 1.798 | 2 | 300 | 50.72 |
| 1.706 | 11 | 310 | 53.67 |
| 1.627 | 12 | 311 | 56.53 |
| 1.538 | 8 | 222 | 59.27 |
| 1.497 | 2 | 320 | 61.95 |
| 1.4421 | 9 | 321 | 64.56 |
| 1.3486 | 2 | 400 | 69.66 |
| 1.3085 | 2 | 410 | 72.72 |
| 1.2717 | 3 | 411 | 74.55 |
| 1.2380 | 2 | 331 | 76.95 |
| 1.2063 | 6 | 420 | 79.36 |
| 1.1505 | 2 | 332 | 84.05 |
| 1.1016 | 4 | 422 | 88.73 |
| 1.0794 | 2 | 500 | 91.06 |
| 1.0583 | 3 | 510 | 93.41 |
| 1.0387 | 2 | 511 | 95.73 |
| 0.9852 | <1 | 521 | 102.85 |
| .9538 | <1 | 440 | 107.72 |
| .9255 | <1 | 530 | 112.66 |
| .9119 | 1 | 531 | 115.27 |
| .8993 | <1 | 600 | 117.85 |
| .8755 | <1 | 611 | 123.23 |
| .8532 | <1 | 620 | 129.05 |
| .8327 | <1 | 541 | 135.35 |
| .8227 | <1 | 533 | 138.86 |
| .8136 | <1 | 622 | 142.43 |

**Powder diffraction cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of cesium copper trichloride was crystallized from an aqueous solution of cesium chloride and cupric chloride. The crystals formed as dark red hexagonal prisms terminated by bipyramids.

Spectrographic analysis showed the major impurities to be 0.01 to 0.1 percent of barium and 0.001 to 0.01 percent each of aluminum, calcium, chromium, iron, potassium, magnesium, manganese, sodium, nickel, rubidium, silicon and strontium.

The color of the sample was very dark red when unground and dark orange yellow when ground. In the petrographic microscope the sample was strongly dichroic, being brownish red for vibrations along c and yellowish for vibrations perpendicular to c. The crystals were uniaxial positive with $N_o = 1.75$ and $N_e = 1.885$.

$I/I_{corundum} = 3.0$.

**Structure data.** Wells (1947) determined that cesium copper trichloride is hexagonal with the space group $D_6^2$-$P6_122$ (No. 178) and 6($CsCuCl_3$) per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Klug and Sears (1946) | 7.189 | 18.06 |
| Wells (1947) | 7.20 | 18.00 |
| NBS, sample at 25°C | 7.2165 ±0.0004 | 18.180 ± 0.002 |

The density of cesium copper trichloride calculated from the NBS lattice constants is 3.679 g/cm³ at 25°C.

## References

Klug, H.P. and Sears, G.W. (1946). A crystal-chemical study of cesium trichlorocuprate, J. Am. Chem. Soc. 68, 1133.

Wells, A.F. (1947). The crystal structure of $CsCuCl_3$ and the crystal chemistry of complex halides $ABX_3$, J. Chem. Soc. (London) 1947, 1662.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 6.249 | 15 | 100 | 14.16 |
| 5.909 | 7 | 101 | 14.98 |
| 4.354 | 75 | 103 | 20.38 |
| 3.676 | 9 | 104 | 24.19 |
| 3.608 | 88 | 110 | 24.65 |
| 3.541 | 12 | 111 | 25.13 |
| 3.146 | 7 | 105 | 28.34 |
| 3.126 | 10 | 200 | 28.53 |
| 3.078 | 8 | 201 | 28.98 |
| 3.032 | 25 | 006 | 29.43 |
| 2.956 | 17 | 202 | 30.21 |
| 2.777 | 100 | 203 | 32.21 |
| 2.726 | 29 | 106 | 32.82 |
| 2.576 | 8 | 204 | 34.80 |
| 2.369 | 9 | 205 | 37.95 |
| 2.319 | 5 | 116 | 38.79 |
| 2.286 | 4 | 212 | 39.38 |
| 2.200 | 17 | 213 | 40.98 |
| 2.175 | 25 | 206 | 41.49 |
| 2.095 | 2 | 214 | 43.14 |
| 2.082 | 10 | 300 | 43.42 |
| 2.070 | 7 | 301 | 43.69 |
| 2.031 | 3 | 302 | 44.58 |
| 1.998 | 7 | 207 | 45.36 |
| 1.981 | 6 | 215 | 45.76 |
| 1.922 | 6 | 109 | 47.24 |
| 1.863 | 11 | 216 | 48.83 |
| 1.805 | 16 | 220 | 50.52 |
| 1.795 | 15 | 221 | 50.81 |
| 1.770 | 3 | 222 | 51.59 |
| 1.747 | 4 | 217 | 52.31 |
| 1.730 | 2 | 223 | 52.89 |
| 1.702 | 11 | 312 | 53.80 |
| 1.697 | 11 | 209 | 53.99 |
| 1.666 | 7 | 313 | 55.08 |
| 1.6163 | 2 | 225 | 56.92 |
| 1.5642 | 5 | 315 | 59.00 |
| 1.5501 | 6 | 226 | 59.59 |
| 1.5396 | 6 | 402 | 60.04 |
| 1.5356 | 5 | 308 | 60.21 |
| 1.5145 | 3 | 0·0·12 | 61.14 |
| 1.5127 | 7 | 403 | 61.22 |
| 1.5040 | 6 | 316 | 61.61 |
| 1.4777 | 6 | 404 | 62.83 |
| 1.4421 | 2 | 317 | 64.57 |

| Internal standard W, a = 3.16504 Å<br>$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d* (Å) | *I* | *hkl* | 2θ(°) |
| 1.4298 | 3 | 321 | 65.19 |
| 1.4163 | 2 | 322 | 65.89 |
| 1.3966 | 5 | 1·1·12 | 66.94 |
| 1.3882 | 5 | 406 | 67.40 |
| 1.3677 | 4 | 324 | 68.55 |
| 1.3637 | 4 | 410 | 68.78 |
| 1.3599 | 5 | 411 | 69.00 |
| 1.3150 | 5 | 319 | 71.71 |

Powder diffraction cards. None.

Additional published patterns. Møller (1959).

NBS sample. The sample of cesium lead trichloride was prepared at NBS by fusion of cesium chloride and lead chloride at about 500° C.

Spectrographic analysis showed the major impurities to be 0.01 to 0.1 percent of potassium and 0.001 to 0.01 percent each of aluminum, barium, calcium, lithium, manganese, sodium, rubidium, silicon and strontium.

The color of the sample was yellow white. Cesium lead trichloride has a very low double refraction. The indices were both near 1.930.

$I/I_{corundum}$ = 8.3.

Structural data. Møller (1959) determined that cesium lead trichloride at room temperature has a distorted perovskite structure, with the tetragonal space group $C_{4v}^{1}$-P4mm (No. 99) and 1 ($CsPbCl_3$) per unit cell. It was also found to go through a readily reversible inversion at 46.9° C, above which it had a cubic pervoskite structure with a = 5.605Å.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Møller (1959) | 5.590 | 5.630 |
| NBS, sample at 25°C | 5.584 ±0.001 | 5.623 ±0.001 |

The density of cesium lead trichloride calculated from the NBS lattice constants is 4.224 g/cm$^3$ at 25° C.

Reference

Møller, C. K. (1959). The structure of perovskite-like cesium plumbo-trihalides, Kgl. Danske Videnskab. Selskab, Mat. fys. Medd. 32 No. 2.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 5.60 | 14 | 100,001 | 15.79 |
| 3.960 | 100 | 101 | 22.43 |
| 2.809 | 14 | 002 | 31.82 |
| 2.794 | 23 | 200 | 32.00 |
| 2.509 | 6 | 102 | 35.75 |
| 2.502 | 7 | 201 | 35.86 |
| 2.288 | 23 | 112 | 39.34 |
| 2.283 | 29 | 211 | 39.43 |
| 1.981 | 10 | 202 | 45.76 |
| 1.976 | 9 | 220 | 45.89 |
| 1.871 | 7 | 003 | 48.62 |
| 1.867 | 9 | 212 | 48.73 |
| 1.862 | 7 | 221,300 | 48.86 |
| 1.777 | 5 | 103 | 51.38 |
| 1.767 | 7 | 301,310 | 51.70 |
| 1.685 | 1 | 311 | 54.39 |
| 1.616 | 3 | 222 | 56.95 |
| 1.557 | <1 | 203 | 59.32 |
| 1.551 | <1 | 302 | 59.54 |
| 1.548 | <1 | 320 | 59.67 |
| 1.4988 | 5 | 213 | 61.85 |
| 1.4949 | 7 | 312 | 62.03 |
| 1.4934 | 5 | 321 | 62.10 |
| 1.4056 | <1 | 004 | 66.46 |
| 1.3965 | <1 | 400 | 66.95 |
| 1.3563 | 1 | 322 | 69.21 |
| 1.3541 | 1 | 401,410 | 69.34 |
| 1.3245 | 1 | 114 | 71.12 |
| 1.3212 | 1 | 303 | 71.32 |
| 1.3168 | 2 | 411 | 71.60 |
| 1.2556 | <1 | 204 | 75.68 |
| 1.2501 | <1 | 402 | 76.07 |
| 1.2253 | <1 | 214 | 77.90 |
| 1.2200 | <1 | 412 | 78.30 |

**Powder Diffraction File cards.** No. 1-0300, Hanawalt, Rinn, and Frevel (1938).

**Additional published patterns.** Thomas (1956).

**NBS sample.** The sample of chromium fluoride trihydrate was obtained from Fisher Scientific Co., Washington, D.C. The sample was recrystallized from a water solution.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of calcium, iron, magnesium, and silicon; and 0.001 to 0.01 percent each of aluminum, manganese, nickel, and lead.

The color of the sample was deep green. Optically it appeared uniaxially positive with indices of refraction $N_\alpha \cong N_\beta = 1.448$ and $N_\gamma = 1.476$. 2V could not be measured.

$I/I_{corundum} = 2.5$.

**Structural data.** Through the help of A. Perloff at this laboratory, single crystal work indicates that the compound is monoclinic with the space group either $C_2^3$-C2 (No. 5) or $C_{2h}^3$-C2/m (No. 12). Visser (1964) was able to give a rhombohedral configuration for this compound. Our data was indexed on both the monoclinic cell and the pseudo-hexagonal cell.

The density of chromium fluoride trihydrate calculated from the NBS lattice constants is 2.236 g/cm³ at 25 °C using $3(CrF_3 \cdot 3H_2O)$ per unit hexagonal cell or $2(CrF_3 \cdot 3H_2O)$ per unit monoclinic cell.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* mono. | hex. | 2θ(°) |
|---|---|---|---|---|
| 4.704 | 100 | 020,111 | 110 | 18.85 |
| 4.101 | 60 | $\bar{1}11$,001 | 101 | 21.65 |
| 3.091 | 4 | 021,$\bar{2}$01 | 021 | 28.86 |
| 2.581 | 53 | $\bar{2}$21,111 | 211 | 34.27 |
| 2.350 | 2 | 040,220,+ | 220 | 38.27 |
| 2.278 | 2 | $\bar{1}$12,$\bar{2}$02 | 012 | 39.52 |
| 2.050 | 8 | $\bar{2}$22,002 | 202 | 44.15 |
| 1.879 | 25 | $\bar{3}$12,022 | 122 | 48.40 |
| 1.871 | 22 | $\bar{2}$41,201 | 401 | 48.61 |
| 1.777 | 9 | 150,240 | 410 | 51.38 |
| 1.738 | 8 | $\bar{3}$31,221 | 321 | 52.60 |
| 1.636 | 14 | $\bar{3}$32,112 | 312 | 56.18 |
| 1.567 | 4 | 060,330 | 330 | 58.87 |
| 1.545 | 4 | 042 | 042 | 59.80 |
| 1.541 | 2 | 151,$\bar{4}$01 | 051 | 59.98 |
| 1.4988 | 4 | $\bar{3}$13,$\bar{1}$13,+ | 113 | 61.85 |
| 1.4675 | 5 | $\bar{1}$52,132,+ | 232 | 63.32 |
| 1.4638 | 4 | 061,241 | 241 | 63.50 |
| 1.3972 | 2 | $\bar{3}$51,311 | 511 | 66.91 |
| 1.3663 | 3 | $\bar{4}$03 | 303 | 68.63 |
| 1.3568 | 2 | 260,400 | 600 | 69.18 |
| 1.3422 | 1 | 202 | 502 | 70.04 |
| 1.3122 | 2 | $\bar{4}$23 | 223 | 71.89 |
| 1.3035 | 4 | 350,$\bar{4}$20 | 520 | 72.44 |
| 1.2907 | 2 | $\bar{3}$42,222 | 422 | 73.28 |
| 1.2450 | 2 | 152 | 152 | 76.44 |
| 1.2013 | 2 | 261,$\bar{5}$11 | 161 | 79.76 |
| 1.1811 | 3 | $\bar{4}$43,113,+ | 413 | 81.41 |
| 1.1738 | 2 | $\bar{3}$14,$\bar{2}$04 | 104 | 82.02 |
| 1.1655 | 2 | $\bar{5}$32 | 342 | 82.73 |
| 1.1389 | 2 | $\bar{1}$81,$\bar{4}$04 | 024 | 85.11 |
| 1.1297 | 2 | $\bar{3}$71,351,+ | 351 | 85.97 |
| 1.1136 | 2 | $\bar{2}$63,133,+ | 333 | 87.53 |

## References


Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Chemical analysis by x-ray diffraction, Ind. Eng. Chem. Anal. Ed. **10**, 457-513.

Thomas, W. G. (1956). The structure of binary crystalline fluorides, Dissertation Abstr. **16**, 467.

Visser, J. W. (1964). (private communication).


*Lattice constants*

| | *a*(Å) | *b*(Å) | *c*(Å) | β(°) |
|---|---|---|---|---|
| Thomas* (hex.) (1956) | 5.41 | --- | 8.31 | --- |
| NBS, sample at 25°C (hex.) | 9.402 | --- | 4.745 | --- |
| NBS, sample at 25°C (mono.) | 6.281 | 9.404 | 4.745 | 120.24° |

*proposed cell does not index pattern.

**Powder Diffraction File cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of cobalt antimony oxide was prepared at NBS by heating a mixture of cobalt oxalate and antimony pentoxide for 1/2 hour at 1000°C on a gold boat.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of chromium, iron, nickel, and silicon; and 0.001 to 0.01 percent each of aluminum, barium, calcium, copper, manganese, molybdenum, vanadium, and zinc.

The color of the sample was light gray brown. The indices of refraction could not be determined because the sample was too fine-grained.

$I/I_{corundum} = 2.5$.

**Structural data.** Byström, Hök, and Mason (1941) determined that cobalt antimony oxide is isomorphous with zinc antimony oxide, with the space group $D_{4h}^{14}$-$P4_2/mnm$ (No. 136) and 2 ($CoSb_2O_6$) per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Byström, Hök, and Mason (1941) | 4.65 | 9.27 |
| NBS, sample at 25°C | 4.6539 | 9.283 |

The density of cobalt antimony oxide calculated from the NBS lattice constants is 6.581 g/cm³ at 25°C.

Internal standard Ag, a = 4.08625 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25°C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 4.643 | 9 | 002 | 19.10 |
| 4.164 | 16 | 101 | 21.32 |
| 3.292 | 100 | 110 | 27.06 |
| 2.686 | 5 | 112 | 33.33 |
| 2.576 | 77 | 103 | 34.80 |
| 2.328 | 20 | 200 | 38.65 |
| 2.254 | 7 | 113 | 39.96 |
| 2.081 | 5 | 210,202 | 43.44 |
| 2.031 | 6 | 211 | 44.58 |
| 1.897 | 2 | 114 | 47.91 |
| 1.726 | 62 | 213 | 53.00 |
| 1.645 | 19 | 220,204 | 55.84 |
| 1.547 | 8 | 006 | 59.73 |
| 1.529 | 2 | 301 | 60.49 |
| 1.472 | 15 | 310 | 63.12 |
| 1.4000 | 16 | 116 | 66.76 |
| 1.3864 | 20 | 303 | 67.50 |
| 1.3422 | 1 | 224 | 70.04 |
| 1.2882 | 6 | 206 | 73.44 |
| 1.2784 | 2 | 321 | 74.10 |
| 1.2754 | 2 | 107 | 74.30 |
| 1.2436 | 2 | 322 | 76.53 |
| 1.2417 | 2 | 216 | 76.68 |
| 1.1914 | 13 | 323 | 80.56 |
| 1.1635 | 3 | 400 | 82.91 |
| 1.1272 | 9 | 226 | 86.21 |
| 1.1207 | 1 | 411 | 86.83 |
| 1.0973 | 4 | 330 | 89.17 |
| 1.0663 | 10 | 316 | 92.50 |
| 1.0606 | 10 | 413 | 93.15 |
| 1.0408 | 5 | 420 | 95.47 |
| 1.0155 | <1 | 422 | 98.66 |
| 1.0070 | 4 | 109 | 99.80 |
| 0.9917 | <1 | 334 | 101.91 |
| .9840 | <1 | 119 | 103.02 |
| .9646 | <1 | 415 | 105.98 |
| .9484 | 2 | 228 | 108.61 |
| .9298 | 6 | 406 | 111.87 |
| .9241 | 12 | 219 | 112.93 |
| .9127 | 5 | 510,432 | 115.11 |
| .9112 | 3 | 318 | 115.40 |
| .8949 | 6 | 336 | 118.80 |
| .8913 | 10 | 503 | 119.58 |
| .8635 | 7 | 426 | 126.26 |
| .8589 | 6 | 309 | 127.47 |
| .8322 | 10 | 523 | 135.49 |
| .8227 | 2 | 440 | 138.87 |
| .8057 | 6 | 329 | 145.87 |
| .7981 | 5 | 530 | 149.64 |
| .7861 | 9 | 516 | 156.96 |

## References

Byström, A., B. Hök, and B. Mason (1941). The crystal structure of zinc metantimonate and similar compounds, Arkiv Kemi, Mineral. Geol. **15B**, No. 4, 1-8.

**Powder Diffraction File cards.** None.

**Additional published patterns.** Byström, Hök, and Mason (1941).

**NBS sample.** The sample of copper antimony oxide was prepared at NBS by a solid state reaction of cupric oxide and antimony pentoxide in a silver boat at 945°C in vacuum for 2 hours.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum, calcium, nickel, silicon, and zinc, and 0.001 to 0.01 percent each of silver, barium, chromium, iron, magnesium, and lead.

The color of the sample was pale yellow green. The indices of refraction could not be determined because the sample was too fine-grained.

$I/1_{corundum} = 4.5$.

**Structural data.** Byström, Hök, and Mason (1941) determined that copper antimony oxide has a deformed trirutile structure, the space group $C_{2h}^5$-$P2_1/n$ (No. 14), and $2(CuSb_2O_6)$ per unit cell.

*Lattice constants*

| | *a*(Å) | *b* (Å) | *c*(Å) | *β*(°) |
|---|---|---|---|---|
| Byström, et.al. (1941) | 4.63 | 4.63 | 9.30 | 91.55° |
| NBS, sample at 25°C | 4.6359 | 4.6339 | 9.294 | 91.14° |

The density of copper antimony oxide calculated from the NBS lattice constants is 6.704 g/cm³ at 25°C.

Internal standard Ag, a = 4.08625 Å
$CuK_{\alpha_1}$ λ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 4.650 | 7 | 002 | 19.07 |
| 4.185 | 7 | $\bar{1}01$ | 21.21 |
| 4.152 | 9 | 011 | 21.38 |
| 4.120 | 6 | 101 | 21.55 |
| 3.274 | 100 | 110 | 27.21 |
| 2.694 | 2 | $\bar{1}12$ | 33.23 |
| 2.660 | 2 | 112 | 33.67 |
| 2.599 | 19 | $\bar{1}03$ | 34.48 |
| 2.576 | 37 | 013 | 34.80 |
| 2.552 | 17 | 103 | 35.13 |
| 2.317 | 21 | 200,020 | 38.83 |
| 2.266 | 3 | $\bar{1}13$ | 39.74 |
| 2.247 | 1 | 021 | 40.09 |
| 2.236 | 3 | 113 | 40.29 |
| 2.073 | 4 | 022 | 43.63 |
| 2.057 | 1 | 202 | 43.98 |
| 2.027 | 2 | $\bar{1}21$ | 44.66 |
| 2.019 | 2 | 121 | 44.85 |
| 2.015 | 2 | 211 | 44.95 |
| 1.909 | 1 | $\bar{1}14,\bar{2}12$ | 47.60 |
| 1.885 | <1 | 122 | 48.23 |
| 1.736 | 17 | $\bar{2}13,\bar{1}05$ | 52.68 |
| 1.730 | 19 | $\bar{1}23$ | 52.88 |
| 1.715 | 17 | 123 | 53.38 |
| 1.709 | 16 | 213 | 53.59 |
| 1.638 | 15 | 220 | 56.08 |
| 1.549 | 8 | 006 | 59.63 |
| 1.539 | 1 | 124 | 60.06 |
| 1.524 | 1 | 031 | 60.72 |
| 1.518 | 1 | 301 | 60.98 |
| 1.4656 | 15 | 310 | 63.41 |
| 1.4078 | 6 | $\bar{1}16$ | 66.34 |
| 1.3998 | 2 | $\bar{1}32$ | 66.77 |
| 1.3928 | 11 | 116 | 67.15 |
| 1.3826 | 8 | 033 | 67.71 |
| 1.3714 | 5 | 215,303 | 68.34 |
| 1.3305 | 1 | 224 | 70.75 |
| 1.2995 | 3 | $\bar{2}06$ | 72.70 |
| 1.2876 | 3 | 026 | 73.48 |
| 1.2759 | 2 | $\bar{3}21,206$ | 74.27 |
| 1.1940 | 4 | $\bar{3}23$ | 80.35 |
| 1.1916 | 5 | $\bar{2}33$ | 80.54 |
| 1.1825 | 5 | 233 | 81.29 |
| 1.1586 | 5 | 400,040 | 83.34 |
| 1.1334 | 6 | $\bar{2}26,\bar{3}24$ | 85.62 |

**Reference**

Byström, A., Hök, B. and Mason, B. (1941). The crystal structure of zinc metantimonate and similar compounds, Arkiv Kemi, Mineral. Geol. 15B, No. 4, 1-8.

| Internal standard Ag, a = 4.08625 Å<br>$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d* (Å) | *I* | *hkl* | 2θ(°) |
| 1.1179 | 5 | 226 | 87.10 |
| 1.0924 | 6 | 330 | 89.68 |
| 1.0747 | 4 | $\bar{3}16$ | 91.57 |
| 1.0680 | 4 | $\bar{1}36$ | 92.31 |
| 1.0629 | 5 | $\bar{2}35$ | 92.88 |
| 1.0614 | 5 | 136 | 93.05 |
| 1.0585 | 6 | $\bar{1}43$ | 93.38 |
| 1.0551 | 8 | 316 | 93.78 |
| 1.0502 | 5 | 413 | 94.35 |
| 1.0363 | 8 | 420,044 | 96.02 |

**Powder Diffraction File cards.** None.

**Additional published patterns.** Milligan, Watt, and Rachford (1949).

**NBS sample.** The sample of erbium vanadate was prepared at NBS. A mixture of erbium oxalate and vanadium pentoxide was heated at 1100°C for 30 minutes.

Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, magnesium, and silicon.

The color of the sample was medium brown. The indices of refraction could not be determined because the sample was too fine-grained.

$I/I_{corundum} = 3.1$.

**Structural data.** Milligan, Watt, and Rachford (1949) determined that erbium vanadate has the zircon structure with the space group $D_{4h}^{19}$-$I4_1/amd$ (No. 141) and 4($ErVO_4$) per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Milligan, Watt, and Rachford (1949) | 7.06* | 6.24 |
| NBS, sample at 25°C | 7.0975 | 6.2723 |

*contains 25% yttrium

The density of erbium vanadate calculated from the NBS lattice constants is 5.932 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 4.704 | 38 | 101 | 18.85 |
| 3.549 | 100 | 200 | 25.07 |
| 2.832 | 12 | 211 | 31.56 |
| 2.660 | 70 | 112 | 33.67 |
| 2.510 | 22 | 220 | 35.74 |
| 2.3504 | 5 | 202 | 38.26 |
| 2.2134 | 18 | 301 | 40.73 |
| 2.0060 | 12 | 103 | 45.16 |
| 1.8783 | 12 | 321 | 48.42 |
| 1.8250 | 58 | 312 | 49.93 |
| 1.7746 | 18 | 400 | 51.45 |
| 1.7461 | 4 | 213 | 52.35 |
| 1.6600 | 4 | 411 | 55.29 |
| 1.5868 | 12 | 420 | 58.08 |
| 1.5676 | 6 | 004 | 58.86 |
| 1.4758 | 15 | 332 | 62.92 |
| 1.4339 | 14 | 204 | 64.98 |
| 1.3842 | 5 | 501 | 67.62 |
| 1.3295 | 12 | 224 | 70.81 |
| 1.2720 | 12 | 512 | 74.53 |
| 1.2546 | 3 | 440 | 75.75 |
| 1.1825 | 5 | 600 | 81.29 |
| 1.1746 | 7 | 404,503 | 81.95 |
| 1.1664 | 3 | 215 | 82.65 |
| 1.1471 | 2 | 611 | 84.36 |
| 1.1345 | 8 | 532 | 85.52 |
| 1.1221 | 5 | 620 | 86.70 |
| 1.1154 | 10 | 424 | 87.35 |
| 1.0580 | 2 | 325 | 93.44 |
| 1.0434 | 1 | 631 | 95.16 |
| 1.0234 | 4 | 116 | 97.63 |
| 1.0190 | 2 | 613 | 98.21 |
| 1.0136 | 2 | 415 | 98.91 |
| 0.9841 | 3 | 640 | 103.01 |
| .9797 | 4 | 444,543 | 103.66 |
| .9634 | 1 | 721 | 106.17 |
| .9560 | 6 | 712 | 107.35 |
| .9478 | 5 | 316 | 108.71 |
| .9443 | 4 | 604,633 | 109.31 |
| .9398 | 2 | 505 | 110.08 |
| .9126 | 6 | 624,703 | 115.14 |
| .8933 | 5 | 732 | 119.15 |
| .8870 | 3 | 800 | 120.55 |
| .8718 | 1 | 811 | 124.13 |
| .8623 | 1 | 217 | 126.57 |
| .8605 | 2 | 820 | 127.05 |
| .8450 | <1 | 714 | 131.45 |
| .8359 | 7 | 660,516 | 134.27 |
| .8335 | 8 | 644,653 | 135.06 |
| .7979 | 5 | 752 | 149.75 |
| .7931 | 6 | 840,536 | 152.45 |

**Reference**

Milligan, W. O., Watt, L. M., and Rachford, H. H., Jr. (1949). X ray diffraction studies of heavy metal orthovanadates, J. Phys. & Colloid Chem. 53, 227-234.

**Powder Diffraction File cards.** None.

**Additional published patterns.** Milligan, Watt, and Rachford (1949), and Nautov (1962).

**NBS sample.** The sample of gadolinium vanadate was prepared at NBS. A mixture of gadolinium oxalate and vanadium pentoxide was heated at 800° C for 15 minutes.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of aluminum, copper, and iron.

The color of the sample was gray yellow. The indices of refraction could not be determined because the sample was too fine-grained.

$I/I_{corundum} = 3.1$.

**Structural data.** Milligan, Watt, and Rachford (1949) determined that gadolinium vanadate has the zircon structure with the space group $D_{4h}^{19}$-$I4_1/amd$ (No. 141) and 4($GdVO_4$) per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Milligan, Watt, and Rachford (1949) | 7.19 | 6.33 |
| Nautov (1962) | 7.196 | 6.345 |
| NBS, sample at 25°C | 7.2126 | 6.3483 |

The density of gadolinium vanadate calculated from the NBS lattice constants is 5.474 g/cm$^3$ at 25° C.

Internal standard W, a = 3.16504 Å

CuK$\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2$\theta$(°) |
|---|---|---|---|
| 4.766 | 28 | 101 | 18.60 |
| 3.606 | 100 | 200 | 24.67 |
| 2.874 | 12 | 211 | 31.09 |
| 2.694 | 76 | 112 | 33.22 |
| 2.551 | 23 | 220 | 35.15 |
| 2.383 | 4 | 202 | 37.71 |
| 2.2482 | 12 | 301 | 40.07 |
| 2.0303 | 10 | 103 | 44.59 |
| 1.9083 | 12 | 321 | 47.61 |
| 1.8520 | 56 | 312 | 49.15 |
| 1.8030 | 16 | 400 | 50.58 |
| 1.7694 | 5 | 213 | 51.61 |
| 1.6865 | 4 | 411 | 54.35 |
| 1.6127 | 12 | 420 | 57.06 |
| 1.5876 | 5 | 004 | 58.05 |
| 1.4986 | 16 | 332 | 61.86 |
| 1.4527 | 14 | 204 | 64.04 |
| 1.4067 | 6 | 501 | 66.40 |
| 1.3476 | 10 | 224 | 69.72 |
| 1.2922 | 12 | 512 | 73.18 |
| 1.2750 | 2 | 440 | 74.33 |
| 1.2020 | 6 | 600 | 79.70 |
| 1.1915 | 8 | 404,503 | 80.55 |
| 1.1813 | 4 | 215 | 81.39 |
| 1.1656 | 3 | 611 | 82.73 |
| 1.1527 | 10 | 532 | 83.86 |
| 1.1404 | 6 | 620 | 84.97 |
| 1.1313 | 10 | 424,523 | 85.82 |
| 1.0602 | 4 | 631 | 93.19 |
| 1.0361 | 8 | 116 | 96.04 |
| 1.0004 | 5 | 640 | 100.70 |
| 0.9942 | 6 | 543,444 | 101.57 |
| .9711 | 8 | 712 | 104.97 |
| .9599 | 4 | 316 | 106.72 |
| .9531 | 4 | 505 | 107.83 |
| .9261 | 6 | 703,624 | 112.55 |
| .9077 | 6 | 732 | 116.12 |
| .8472 | 8 | 516 | 130.78 |
| .8107 | 6 | 752 | 143.65 |
| .8040 | 10 | 536 | 146.66 |
| .7840 | 6 | 833,804 | 158.54 |

## References

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Nautov, V.A. (1962). X-ray study of scandium, yttrium, cerium, neodymium, and gadolinium orthovanadates, Zh. Strukt. Khim. 3, 608-611.

**Powder diffraction card.** No. 11-614, Basta (1957).

**Additional published patterns.** Holgersson (1927), Jung and Köhler (1930), and Hanawalt, Rinn, and Frevel (1938).

**NBS sample.** The sample of iron(II,III) oxide was obtained from the Columbian Carbon Co., New York 17, N.Y.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent cobalt and 0.001 to 0.01 percent each of silver, aluminum, magnesium, manganese, molybdenum, nickel, silicon, titanium, and zinc.

The sample was a black opaque powder.

$I/I_{corundum} = 4.9$.

**Structural data.** Bragg (1915) determined that iron(II,III) oxide has the spinel structure, the space group $O_h^7$-Fd3m (No. 227) and 8($Fe_3O_4$) per unit cell.

*Lattice constants*

| | *a*(Å) |
|---|---|
| Goldschmidt (1942) | 8.43 |
| Lindroth (1946) | 8.416 |
| Mason (1947) | 8.398 |
| Pouillard (1950) | 8.413 |
| Tombs and Rooksby (1951), sample at 22°C. | 8.3940 |
| Abrahams and Calhoun (1953) sample at 22°C. | 8.3940 |
| Yearian et al. (1954) metal rich | 8.396 |
| Yearian et al. (1954) oxygen rich | 8.390 |
| Radavich (1955) | 8.394 |
| Basta (1957), sample at 18°C. | 8.3963 |
| NBS, sample at 25°C. | 8.396 |

The density of iron(II,III) oxide calculated from the NBS lattice constant is 5.197 g/cm$^3$ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2$\theta$(°) | *a* (Å) |
|---|---|---|---|---|
| 4.852 | 8 | 111 | 18.27 | 8.40 |
| 2.967 | 28 | 220 | 30.09 | 8.393 |
| 2.532 | 100 | 311 | 35.42 | 8.398 |
| 2.4243 | 7 | 222 | 37.05 | 8.398 |
| 2.0993 | 21 | 400 | 43.05 | 8.397 |
| 1.7146 | 10 | 422 | 53.39 | 8.400 |
| 1.6158 | 27 | 511 | 56.94 | 8.396 |
| 1.4845 | 41 | 440 | 62.51 | 8.398 |
| 1.4192 | 2 | 531 | 65.74 | 8.396 |
| 1.3277 | 4 | 620 | 70.92 | 8.397 |
| 1.2807 | 9 | 533 | 73.95 | 8.398 |
| 1.2659 | 4 | 622 | 74.96 | 8.397 |
| 1.2119 | 2 | 444 | 78.93 | 8.396 |
| 1.1221 | 3 | 642 | 86.70 | 8.397 |
| 1.0930 | 12 | 731 | 89.61 | 8.396 |
| 1.0496 | 5 | 800 | 94.42 | 8.397 |
| 0.9896 | 2 | 822 | 102.21 | 8.397 |
| .9695 | 6 | 751 | 105.21 | 8.396 |
| .9632 | 3 | 662 | 106.20 | 8.397 |
| .9388 | 3 | 840 | 110.27 | 8.397 |
| .8952 | 2 | 664 | 118.73 | 8.398 |
| .8802 | 5 | 931 | 122.09 | 8.397 |
| .8569 | 7 | 844 | 128.03 | 8.396 |
| .8233 | 3 | 10.2.0 | 138.63 | 8.396 |
| .8117 | 6 | 951 | 143.23 | 8.396 |
| .8080 | 4 | 10.2.2 | 144.82 | 8.397 |

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**Powder Diffraction File cards.** No. 6-0330, Lamb and Niebylski (1953), and No. 6-0412, Thornton Research Centre, The Shell Petroleum Co., Ltd. (1954).

**Additional published patterns.** None.

**NBS sample.** The sample of lead oxybromide was prepared at NBS from red lead monoxide and lead bromide. A stoichiometric mixture was placed on gold leaf, sealed in an evacuated tube, and heated 3/4 hr. at 350°C.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of bismuth, molybdenum, silicon, and strontium, and 0.001 to 0.01 percent each of alumunim, barium, calcium, chromium, copper, iron, sodium, nickel, titanium, and vanadium.

The color of the sample was yellow white. The indices of refraction could not be determined because the sample was too fine-grained

$I/I_{corundum} = 1.3$.

**Structural data.** Davies (1957) determined that lead oxybromide has the space group $D_{2h}^{16}$-Pbnm (No. 62), and 4($Pb_3O_2Br_2$) per unit cell.

*Lattice constants*

| | *a*(Å) | *b*(Å) | *c*(Å) |
|---|---|---|---|
| Thornton Research Centre (1954) | 9.7 | 12.1 | 5.88 |
| Davies (1957) | 9.81 | 12.25 | 5.88 |
| NBS, sample at 25°C | 9.8162 | 12.253 | 5.8754 |

The density of lead oxybromide calculated from the NBS lattice constants is 7.645 g/cm³ at 25°C.

Internal standard Ag, a = 4.08625 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 7.67 | 54 | 110 | 11.53 |
| 5.20 | 23 | 120 | 17.03 |
| 4.91 | 7 | 200 | 18.06 |
| 4.66 | 2 | 111 | 19.04 |
| 4.241 | 6 | 021 | 20.93 |
| 3.895 | 39 | 121 | 22.81 |
| 3.771 | 3 | 130 | 23.57 |
| 3.600 | 48 | 211 | 24.71 |
| 3.172 | 75 | 131 | 28.11 |
| 3.139 | 64 | 230 | 28.41 |
| 2.937 | 95 | 002 | 30.41 |
| 2.857 | 92 | 301 | 31.28 |
| 2.783 | 40 | 311 | 32.14 |
| 2.715 | 100 | 041 | 32.96 |
| 2.597 | 9 | 240 | 34.50 |
| 2.591 | 9 | 321 | 34.59 |
| 2.554 | 13 | 330 | 35.11 |
| 2.522 | 3 | 202 | 35.57 |
| 2.454 | 4 | 400 | 36.59 |
| 2.376 | 11 | 241 | 37.84 |
| 2.317 | 2 | 132 | 38.83 |
| 2.278 | 7 | 420 | 39.53 |
| 2.236 | 28 | 340 | 40.29 |
| 2.145 | 43 | 232 | 42.09 |
| 2.124 | 7 | 421 | 42.53 |
| 2.058 | 4 | 322 | 43.95 |
| 2.042 | 6 | 060 | 44.32 |
| 2.000 | 4 | 160 | 45.31 |
| 1.962 | 5 | 350 | 46.24 |
| 1.938 | 10 | 510 | 46.83 |
| 1.927 | 9 | 332 | 47.11 |
| 1.861 | 7 | 412,351 | 48.90 |
| 1.842 | 5 | 511 | 49.44 |
| 1.833 | 6 | 123 | 49.69 |
| 1.822 | 3 | 441 | 50.03 |
| 1.800 | 12 | 422,213 | 50.67 |
| 1.779 | 29 | 342 | 51.30 |
| 1.738 | 9 | 133 | 52.61 |
| 1.724 | 9 | 170 | 53.08 |
| 1.694 | 16 | 531 | 54.08 |
| 1.680 | 18 | 303 | 54.57 |
| 1.663 | 14 | 451 | 55.19 |
| 1.650 | 20 | 043 | 55.65 |
| 1.631 | 7 | 352 | 56.36 |
| 1.621 | 8 | 610,323 | 56.73 |

## References


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Thornton Research Centre, The Shell Petroleum Co., Ltd. (1954), **X-ray Diffraction Patterns of Lead Compounds**, 34-35.

| Internal standard Ag, a = 4.08625 Å<br>$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d* (Å) | *I* | *hkl* | 2θ(°) |
| 1.6182 | 9 | 512 | 56.85 |
| 1.5878 | 16 | 271 | 58.04 |
| 1.5637 | 3 | 243,611 | 59.02 |
| 1.5314 | 4 | 080 | 60.39 |
| 1.5265 | 3 | 621 | 60.61 |
| 1.5167 | 5 | 461 | 61.04 |
| 1.4921 | 3 | 371,362 | 62.16 |
| 1.4865 | 5 | 172 | 62.42 |
| 1.4694 | 11 | 004 | 63.23 |
| 1.4200 | 5 | 612 | 65.70 |

**Powder Diffraction File cards.** No. 8-108 (natural), Claringbull and No. 8-476 (1957) National Bureau of Standards. These new NBS data are essentially the same as reported by us on card No. 8-476. However, the x-ray pattern was rerun to pick up additional weak lines which slower diffractometer scanning brought out.

**NBS sample.** This sample was also prepared by precipitation of solutions of lead nitrate and sodium tungstate.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of aluminum, chromium, iron, and molybdenum.

The color of the sample was very pale yellow white. The indices of refraction could not be determined because the sample was too fine-grained.

$I/I_{corundum} = 8.3$.

**Structural data.** Vegard and Refsum (1928) determined that stolzite has the calcium tungstate structure, the space group $C^6_{4h}$-$I4_1/a$ (No. 88) and $4(PbWO_4)$ per unit cell. Shaw and Claringbull (1955) reported that the monoclinic lead tungstate, raspite, transforms irreversibly to stolzite at about 400°C.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| NBS (1957), sample at 25°C | 5.4616 | 12.046 |
| NBS, sample at 25°C | 5.4619 | 12.049 |

The density of stolzite calculated from the NBS lattice constants is 8.408 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 3.248 | 100 | 112 | 27.44 |
| 3.012 | 22 | 004 | 29.63 |
| 2.732 | 32 | 200 | 32.75 |
| 2.489 | <1 | 202 | 36.05 |
| 2.395 | 1 | 211 | 37.52 |
| 2.376 | 2 | 114 | 37.83 |
| 2.205 | 1 | 105 | 40.89 |
| 2.087 | 2 | 213 | 43.31 |
| 2.024 | 35 | 204 | 44.73 |
| 1.931 | 16 | 220 | 47.01 |
| 1.838 | <1 | 222 | 49.55 |
| 1.7997 | <1 | 301 | 50.68 |
| 1.7820 | 21 | 116 | 51.22 |
| 1.6606 | 33 | 312 | 55.27 |
| 1.6258 | 16 | 224 | 56.56 |
| 1.5065 | 3 | 008 | 61.50 |
| 1.4175 | <1 | 323 | 65.83 |
| 1.3656 | 4 | 400 | 68.67 |
| 1.3187 | 7 | 208 | 71.48 |
| 1.3093 | 11 | 316 | 72.07 |
| 1.2588 | 6 | 332 | 75.45 |
| 1.2436 | 5 | 404 | 76.54 |
| 1.2213 | 5 | 420 | 78.20 |
| 1.1876 | 5 | 228 | 80.87 |
| 1.1501 | 4 | 1·1·10 | 84.09 |
| 1.1318 | 7 | 424 | 85.77 |
| 1.0838 | 4 | 336 | 90.58 |
| 1.0547 | 6 | 512 | 93.82 |
| 1.0115 | 3 | 408 | 99.19 |
| 1.0039 | 1 | 0·0·12 | 100.21 |
| 0.9881 | 6 | 3·1·10 | 102.43 |
| .9655 | 1 | 440 | 105.83 |
| .9486 | 3 | 428 | 108.58 |
| .9451 | 5 | 516 | 109.17 |
| .9424 | 2 | 2·0·12 | 109.63 |
| .9256 | 4 | 532 | 112.65 |
| .9194 | 2 | 444 | 113.81 |
| .9105 | 1 | 600 | 115.55 |
| .8908 | 3 | 2·2·12 | 119.69 |
| .8796 | 3 | 3·3·10 | 122.24 |
| .8714 | 3 | 604 | 124.24 |
| .8636 | 3 | 620 | 126.23 |
| .8489 | 5 | 536 | 130.29 |
| .8400 | 3 | 1·1·14 | 132.97 |
| .8301 | 5 | 624 | 136.21 |
| .8128 | 2 | 448 | 142.75 |
| .8089 | 3 | 4·0·12 | 144.44 |
| .8005 | 5 | 5·1·10 | 148.38 |
| .7790 | 3 | 608 | 162.78 |

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**Powder diffraction cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of lithium barium trifluoride was made at NBS by fusing stoichiometric amounts of anhydrous lithium and barium fluorides at approximately 800°C, and annealing at 500°C for several hours to react with the small percent of $BaF_2$ which formed because of the incongruent crystallization of $LiBaF_3$.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent strontium; 0.01 to 0.1 percent aluminum; and 0.001 to 0.01 percent each of iron, sodium, rubidium, silicon, and titanium.

The sample was almost colorless. The index of refraction was 1.544.

$I/I_{corundum}$ = 0.8.

**Structural data.** Ludekens and Welch (1952) reported that lithium barium trifluoride has an undistorted "inverted" perovskite structure with the space group $O_h^1$-Pm3m (No. 221) and 1 ($LiBaF_3$) per unit cell.

*Lattice constants*

| | *a*(Å) |
|---|---|
| Ludekens and Welch (1952)------ | 3.996 |
| NBS, sample at 25°C---------- | 3.9950 |

The density of lithium barium trifluoride calculated from the NBS lattice constant is 5.242 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) | *a* (Å) |
|---|---|---|---|---|
| 3.994 | 100 | 100 | 22.24 | 3.994 |
| 2.823 | 85 | 110 | 31.67 | 3.992 |
| 2.307 | 83 | 111 | 39.01 | 3.996 |
| 1.997 | 47 | 200 | 45.38 | 3.994 |
| 1.7868 | 34 | 210 | 51.07 | 3.9956 |
| 1.6307 | 30 | 211 | 56.37 | 3.9944 |
| 1.4123 | 20 | 220 | 66.10 | 3.9946 |
| 1.3318 | 15 | 300 | 70.67 | 3.9954 |
| 1.2633 | 11 | 310 | 75.14 | 3.9949 |
| 1.2044 | 17 | 311 | 79.51 | 3.9945 |
| 1.1531 | 6 | 222 | 83.82 | 3.9945 |
| 1.1080 | 5 | 320 | 88.08 | 3.9949 |
| 1.0676 | 10 | 321 | 92.35 | 3.9946 |
| 0.9986 | 5 | 400 | 100.95 | 3.9943 |
| .9689 | 8 | 410 | 105.30 | 3.9950 |
| .9417 | 7 | 411 | 109.74 | 3.9952 |
| .9165 | 8 | 331 | 114.37 | 3.9949 |
| .8934 | 6 | 420 | 119.13 | 3.9952 |
| .8718 | 5 | 421 | 124.15 | 3.9949 |
| .8516 | 6 | 332 | 129.50 | 3.9946 |
| .8155 | 8 | 422 | 141.63 | 3.9953 |
| .7990 | 5 | 500 | 149.15 | 3.9951 |
| .7835 | 13 | 510 | 158.88 | 3.9951 |

## Reference

Ludekens, W.L.W. and Welch, A.J.E. (1952). Reactions between metal oxides and fluorides: some new double-fluoride structures of type $ABF_3$, Acta Cryst 5, 841.

**Powder Diffraction File cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of lutetium arsenate was prepared at NBS from lutetium oxide and arsenic trioxide. The mixture was heated 1 hr. at 1050°C. Later it was heated again for 1 hr. at 1250°C.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent silicon; 0.01 to 0.1 percent each of aluminum and calcium; and 0.001 to 0.01 percent each of copper, iron, magnesium, nickel, lead, antimony, and titanium.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine-grained.

$I/I_{corundum} = 6.4$.

**Structural data.** No reference to the structure of lutetium arsenate was found, but it is apparently isostructural with yttrium arsenate with the space group $D_{4h}^{19}$-$I4_1/amd$ (No. 141) and $4(LuAsO_4)$ per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| NBS, sample at 25°C | 6.9509 | 6.2321 |

The density of lutetium arsenate calculated from the NBS lattice constants is 6.924 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2*θ*(°) |
|---|---|---|---|
| 4.643 | 22 | 101 | 19.10 |
| 3.477 | 100 | 200 | 25.60 |
| 2.783 | 6 | 211 | 32.14 |
| 2.632 | 73 | 112 | 34.03 |
| 2.458 | 25 | 220 | 36.53 |
| 2.321 | 3 | 202 | 38.77 |
| 2.172 | 10 | 301 | 41.54 |
| 1.991 | 6 | 103 | 45.52 |
| 1.8422 | 8 | 321 | 49.43 |
| 1.7964 | 57 | 312 | 50.78 |

continued

| *d* (Å) | *I* | *hkl* | 2*θ*(°) |
|---|---|---|---|
| 1.7375 | 16 | 400 | 52.63 |
| 1.7275 | 2 | 213 | 52.96 |
| 1.6271 | 2 | 411 | 56.51 |
| 1.5578 | 6 | 004 | 59.27 |
| 1.5541 | 15 | 420 | 59.42 |
| 1.4499 | 15 | 332 | 64.18 |
| 1.4215 | 12 | 204 | 65.62 |
| 1.4131 | <1 | 323 | 66.06 |
| 1.3568 | 3 | 501 | 69.18 |
| 1.3158 | 9 | 224 | 71.66 |
| 1.3092 | 1 | 413 | 72.08 |
| 1.2489 | 13 | 512 | 76.16 |
| 1.2287 | 3 | 440 | 77.64 |
| 1.1598 | 5 | 404 | 83.23 |
| 1.1584 | 3 | 600 | 83.35 |
| 1.1239 | <1 | 611 | 86.52 |
| 1.1135 | 9 | 532 | 87.54 |
| 1.1002 | 11 | 424 | 88.87 |
| 1.0468 | <1 | 325 | 94.75 |
| 1.0221 | <1 | 631 | 97.81 |
| 1.0162 | 4 | 116 | 98.57 |
| 1.0017 | <1 | 415,613 | 100.52 |
| 0.9806 | <1 | 701 | 103.53 |
| .9643 | 5 | 444,640 | 106.02 |
| .9621 | 4 | 543 | 106.38 |
| .9438 | <1 | 721 | 109.40 |
| .9390 | 7 | 316 | 110.22 |
| .9374 | 10 | 712 | 110.51 |
| .9296 | 3 | 604 | 111.90 |
| .8981 | 6 | 624 | 118.11 |
| .8771 | 3 | 336 | 122.84 |
| .8758 | 6 | 732 | 123.15 |
| .8689 | 1 | 800 | 124.87 |
| .8559 | <1 | 217 | 128.29 |
| .8540 | 1 | 741 | 128.83 |
| .8428 | 3 | 820 | 132.10 |
| .8262 | 7 | 516 | 137.60 |
| .8197 | 6 | 644 | 140.00 |
| .8082 | <1 | 327 | 144.72 |
| .8065 | <1 | 831 | 145.53 |
| .7964 | <1 | 743 | 150.57 |
| .7873 | <1 | 417 | 156.13 |
| .7831 | 7 | 536 | 159.25 |

**Powder Diffraction File cards.** None.

**Additional published patterns.** Milligan, Watt, and Rachford (1949).

**NBS sample.** The sample of lutetium vanadate was prepared at NBS by precipitation from a solution of sodium vanadate and lutetium sulfate. It was annealed 15 hours at 1300°C.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of calcium and silicon and 0.001 to 0.01 percent each of aluminum, cobalt, iron, magnesium, and tin.

The color of the sample was yellow white. The indices of refraction could not be determined because the sample was too fine-grained.

$I/I_{corundum} = 3.7$.

**Structural data.** Milligan, Watt, and Rachford (1949) determined that lutetium vanadate has the zircon structure, with the space group $D_{4h}^{19}$-$I4_1/amd$ (No. 141) and 4($LuVO_4$) per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Milligan, Watt, and Rachford (1949) | 7.00 | 6.21 |
| NBS, sample at 25°C | 7.0243 | 6.2316 |

The density of lutetium vanadate calculated from the NBS lattice constants is 6.262 g/cm³ at 25°C.

**Reference**

Milligan, W. O., Watt, L. M., and Rachford, H. H., Jr. (1949). X-ray diffraction studies of heavy metal orthovanadates, J. Phys. & Colloid Chem. 53, 227-234.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 4.660 | 41 | 101 | 19.03 |
| 3.510 | 100 | 200 | 25.35 |
| 2.805 | 12 | 211 | 31.88 |
| 2.640 | 65 | 112 | 33.92 |
| 2.483 | 17 | 220 | 36.15 |
| 2.330 | 3 | 202 | 38.60 |
| 2.191 | 14 | 301 | 41.16 |
| 1.9918 | 9 | 103 | 45.50 |
| 1.8592 | 9 | 321 | 48.95 |
| 1.8090 | 43 | 312 | 50.40 |

continued

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 1.7558 | 13 | 400 | 52.04 |
| 1.7323 | 3 | 213 | 52.80 |
| 1.6434 | 4 | 411 | 55.90 |
| 1.5702 | 10 | 420 | 58.75 |
| 1.5580 | 3 | 004 | 59.26 |
| 1.5544 | | 303 | 59.41 |
| 1.4621 | 11 | 332 | 63.58 |
| 1.4240 | 9 | 204 | 65.49 |
| 1.3703 | 12 | 501 | 68.40 |
| 1.3194 | 7 | 224 | 71.43 |
| 1.3171 | | 413 | 71.58 |
| 1.2763 | 3 | 521 | 74.24 |
| 1.2598 | 10 | 512 | 75.38 |
| 1.2417 | 2 | 440 | 76.68 |
| 1.1708 | 3 | 600 | 82.28 |
| 1.1638 | 5 | 503 | 82.88 |
| 1.1354 | <1 | 611 | 85.44 |
| 1.1238 | 6 | 532 | 86.53 |
| 1.1106 | 3 | 620 | 87.82 |
| 1.1061 | 6 | 424 | 88.27 |
| 1.0806 | 2 | 541 | 90.93 |
| 1.0499 | <1 | 325 | 94.38 |
| 1.0326 | <1 | 631 | 96.47 |
| 1.0167 | 2 | 116 | 98.50 |
| 1.0093 | 1 | 613 | 99.48 |
| 1.0058 | 1 | 415 | 99.95 |
| 0.9908 | <1 | 701 | 102.05 |
| .9742 | 1 | 640 | 104.49 |
| .9712 | 1 | 444 | 104.95 |
| .9535 | 1 | 721 | 107.76 |
| .9465 | 4 | 712 | 108.93 |
| .9409 | 3 | 316 | 109.89 |
| .9360 | 1 | 604 | 110.76 |
| .9326 | <1 | 505 | 111.36 |
| .9044 | 3 | 624 | 116.79 |
| .8844 | 2 | 732 | 121.13 |
| .8800 | 1 | 336 | 122.16 |
| .8780 | <1 | 800 | 122.64 |
| .8750 | <1 | 723 | 123.36 |
| .8630 | <1 | 811 | 126.39 |
| .8567 | 1 | 217 | 128.08 |
| .8519 | 2 | 820 | 129.41 |
| .8294 | 2 | 516 | 136.46 |
| .8259 | 3 | 644 | 137.68 |
| .8151 | <1 | 831 | 141.81 |
| .8097 | <1 | 327 | 144.07 |
| .8034 | <1 | 813 | 146.95 |
| .7897 | 5 | 752 | 154.50 |
| .7868 | 3 | 536 | 156.46 |
| .7853 | 3 | 840 | 157.51 |

**Powder diffraction cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of potassium cadmium trichloride was prepared at NBS by melting potassium chloride and cadmium chloride (2 1/2 hydrate) at 550°C. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, barium, chromium, iron, manganese, sodium, rubidium, and strontium.

The sample was colorless and optically positive with a small 2V. The refractive indices were $N_\alpha = 1.700$, $N_\beta = 1.708$, and $N_\gamma = 1.742$.

$I/I_{corundum} = 1.8$.

**Structural data.** Brandenberger (1947) reported that potassium cadmium trichloride is isostructural with ammonium cadmium trichloride, with the space group $D_{2h}^{16}$-Pnam (No. 62) and 4($KCdCl_3$) per unit cell.

*Lattice constants*

| | *a*(Å) | *b*(Å) | *c*(Å) |
|---|---|---|---|
| Brandenberger (1947)------ | 8.78 | 14.56 | 3.99 |
| NBS, sample at 25°C-------- | 8.785 ±0.001 | 14.584 ±0.001 | 3.9969 ±0.0004 |

The density of potassium cadmium trichloride calculated from the NBS lattice constants is 3.345 g/cm³ at 25°C.

## Reference

Brandenberger, E. (1947). Die Kristallstruktur von $K(CdCl_3)$, Experientia 3, 149.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 7.52 | 62 | 110 | 11.75 |
| 7.28 | 79 | 020 | 12.14 |
| 5.615 | 60 | 120 | 15.77 |
| 4.396 | 16 | 200 | 20.18 |
| 4.253 | 17 | 130 | 20.87 |
| 4.209 | 17 | 210 | 21.09 |
| 3.760 | 15 | 220 | 23.64 |
| 3.648 | 6 | 040 | 24.38 |
| 3.531 | 64 | 111 | 25.20 |
| 3.368 | 27 | 140 | 26.44 |
| 3.259 | 34 | 230,121 | 27.34 |
| 3.086 | 9 | 031 | 28.91 |
| 2.956 | 24 | 201 | 30.21 |
| 2.897 | 52 | 211 | 30.84 |
| 2.871 | 7 | 310 | 31.12 |
| 2.806 | 19 | 240 | 31.87 |
| 2.768 | 29 | 150 | 32.31 |
| 2.740 | 100 | 221 | 32.65 |
| 2.718 | 20 | 320 | 32.92 |
| 2.526 | 15 | 231 | 35.51 |
| 2.509 | 7 | 330 | 35.76 |
| 2.429 | 13 | 060,250 | 36.97 |
| 2.356 | 40 | 051 | 38.17 |
| 2.343 | 26 | 160 | 38.39 |
| 2.295 | 5 | 241 | 39.22 |
| 2.283 | 4 | 340 | 39.44 |
| 2.125 | 3 | 331 | 42.51 |
| 2.103 | 3 | 420 | 42.98 |
| 2.076 | 7 | 251 | 43.55 |
| 2.068 | 7 | 350 | 43.74 |
| 2.026 | 9 | 170 | 44.68 |
| 2.021 | 11 | 161 | 44.81 |
| 1.998 | 36 | 002 | 45.34 |
| 1.982 | 32 | 341 | 45.73 |
| 1.925 | 13 | 401 | 47.17 |
| 1.882 | 13 | 122,270,+ | 48.32 |
| 1.879 | 11 | 261 | 48.41 |
| 1.870 | 10 | 360 | 48.65 |
| 1.860 | 13 | 421 | 48.92 |
| 1.8478 | 6 | 071 | 49.27 |
| 1.8232 | 5 | 080 | 49.98 |
| 1.8077 | 23 | 132,171 | 50.44 |
| 1.7892 | 5 | 431 | 51.00 |
| 1.7650 | 4 | 222 | 51.75 |
| 1.7546 | 8 | 450 | 52.08 |

| Internal standard W, a = 3.16504 Å<br>$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d (Å)* | *I* | *hkl* | *2θ(°)* |
| 1.7446 | 4 | 510 | 52.40 |
| 1.7187 | 6 | 142 | 53.25 |
| 1.7077 | 8 | 520 | 53.62 |
| 1.7030 | 10 | 232,271,+ | 53.78 |
| 1.6975 | 7 | 370 | 53.97 |
| 1.6940 | 3 | 361 | 54.09 |
| 1.6839 | 2 | 280 | 54.44 |
| 1.6404 | 3 | 312 | 56.01 |
| 1.6292 | 7 | 460,181 | 56.43 |
| 1.6205 | 5 | 152 | 56.76 |
| 1.5825 | 2 | 540 | 58.25 |
| 1.5625 | 2 | 332,371 | 59.07 |
| 1.5438 | 4 | 062,252 | 59.86 |
| 1.5271 | 5 | 531 | 60.58 |
| 1.5205 | 7 | 290,162 | 60.87 |
| 1.5056 | 3 | 550 | 61.54 |
| 1.5034 | 4 | 342 | 61.64 |
| 1.4805 | 4 | 191 | 62.70 |
| 1.4719 | 4 | 541 | 63.11 |
| 1.4644 | 2 | 600 | 63.47 |
| 1.4383 | 6 | 1·10·0 | 64.76 |
| 1.4355 | 8 | 620 | 64.90 |
| 1.4240 | 6 | 560 | 65.49 |
| 1.4180 | 10 | 390 | 65.80 |

**Powder Diffraction File cards.** None.

**Additional published patterns.** Milligan, Watt, and Rachford (1949).

**NBS sample.** The sample of praseodymium vanadate was prepared at NBS. A mixture of praseodymium oxalate and vanadium pentoxide was heated at 850°C for 30 minutes.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum and silicon, and 0.001 to 0.01 percent each of silver, iron, and magnesium.

The color of the sample was gray green yellow. The indices of refraction could not be determined because the sample was too fine-grained.

$I/I_{corundum} = 3.2$.

**Structural data.** Milligan, Watt, and Rachford (1949) determined that praseodymium vanadate has the zircon structure with the space group $D_{4h}^{19}$ -$I4_1/amd$ (No. 141) and 4($PrVO_4$) per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Milligan, Watt, and Rachford (1949) | 7.29 | 6.41 |
| Vickery and Klann (1957) | 7.31 | 6.45 |
| Schwarz (1963) | 7.367 | 6.468 |
| NBS, sample at 25°C | 7.3633 | 6.4652 |

The density of praseodymium vanadate calculated from the NBS lattice constants is 4.848 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 4.862 | 28 | 101 | 18.23 |
| 3.682 | 100 | 200 | 24.15 |
| 2.936 | 10 | 211 | 30.42 |
| 2.747 | 68 | 112 | 32.57 |
| 2.604 | 22 | 220 | 34.41 |
| 2.430 | 4 | 202 | 36.96 |
| 2.295 | 16 | 301 | 39.22 |
| 2.069 | 10 | 103 | 43.71 |
| 1.947 | 10 | 321 | 46.60 |
| 1.889 | 53 | 312 | 48.11 |
| 1.841 | 16 | 400 | 49.47 |
| 1.803 | 4 | 213 | 50.58 |
| 1.721 | 3 | 411 | 53.17 |
| 1.647 | 12 | 420 | 55.78 |
| 1.620 | 5 | 303 | 56.78 |
| 1.617 | 5 | 004 | 56.91 |
| 1.529 | 12 | 332 | 60.49 |
| 1.480 | 12 | 204 | 62.70 |
| 1.435 | 5 | 501 | 64.92 |
| 1.373 | 9 | 224 | 68.23 |
| 1.318 | 12 | 512 | 71.50 |
| 1.3011 | 3 | 440 | 72.60 |
| 1.2272 | 35 | 600 | 77.75 |
| 1.2150 | 8 | 404 | 78.69 |
| 1.2036 | 3 | 215 | 79.58 |
| 1.1901 | 2 | 611 | 80.66 |
| 1.1763 | 7 | 532 | 81.81 |
| 1.1644 | 5 | 620 | 82.83 |
| 1.1535 | 8 | 424 | 83.79 |
| 1.0929 | 2 | 325 | 89.62 |
| 1.0822 | 2 | 631 | 90.75 |
| 1.0553 | 6 | 613,116 | 93.75 |
| 1.0475 | 1 | 415 | 94.67 |
| 1.0214 | 2 | 640 | 97.90 |
| 1.0140 | 2 | 444 | 98.85 |
| 0.9912 | 6 | 712 | 101.99 |
| .9779 | 6 | 633,316 | 103.94 |
| .9448 | 4 | 624 | 109.23 |
| .9264 | 4 | 732 | 112.49 |
| .9157 | 3 | 336,723 | 114.52 |
| .8931 | 3 | 820 | 119.19 |
| .8636 | 10 | 653,516 | 126.24 |
| .8412 | 2 | 327,813 | 132.61 |
| .8275 | 2 | 752 | 137.14 |
| .8198 | 3 | 536 | 139.96 |
| .7999 | 3 | 833,804 | 148.72 |
| .7893 | 4 | 208 | 154.76 |
| .7887 | 3 | 912 | 155.19 |

## References


Milligan, W. O., Watt, L. M. and Rachford, H. H., Jr. (1949). X-ray diffraction studies of heavy metal orthovanadates, J. Phys. & Colloid Chem. 53, 227-234.

Schwarz, H. (1963). Uber die Chromate(V) der Seltenen Erden, II. Praseodymchromat(V) $PrCrO_4$, Z. anorg. u allgem. Chem. 322, 15-24.

Vickery, R. C. and Klann, A. (1957). Magnetic susceptibilities of vanadates of neodymium and praseodymium, J. Chem. Phys. 27, 1219.

**Powder diffraction cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of rubidium cadmium trichloride was precipitated at NBS from solutions of rubidium chloride and cadmium chloride.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of cesium and potassium; 0.01 to 0.1 percent sodium; and 0.001 to 0.01 percent each of aluminum, barium, calcium, chromium, copper, iron, nickel, silicon, and strontium.

The sample was colorless and optically positive with a very small 2V. The refractive indices were $N_\alpha = 1.694$, $N_\beta = 1.696$, and $N_\gamma = 1.736$. $I/I_{corundum} = 2.2$.

**Structural data.** MacGillavry, Nijveld, Dierdorp, and Karsten (1939) determined that orthorhombic rubidium cadmium trichloride is isostructural with ammonium cadmium trichloride, with the space group $D_{2h}^{16}$-Pnam (No. 62) and 4($RbCdCl_3$) per unit cell. In recent work here, two high temperature forms were also observed for rubidium cadmium trichloride. Between 135°C and 190°C a tetragonal phase exists which persists at room temperature for a day or two. Above 190°C a cubic form was noted on the hot stage of a microscope. This cubic form reverts to tetragonal again below 190°C.

*Lattice constants*

| | *a*(Å) | *b*(Å) | *c*(Å) |
|---|---|---|---|
| MacGillavry, et al. (1939)---- | 9.03 | 14.96 | 4.02 |
| NBS, sample at 25°C--------- | 8.959 ±0.001 | 14.976 ±0.002 | 4.0346 ±0.0004 |

The density of orthorhombic rubidium cadmium trichloride calculated from the NBS lattice constants is 3.733 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 7.67 | 28 | 110 | 11.52 |
| 7.47 | 34 | 020 | 11.83 |
| 5.741 | 25 | 120 | 15.42 |
| 4.480 | 5 | 200 | 19.80 |
| 4.358 | 45 | 130 | 20.36 |
| 4.289 | 32 | 210 | 20.69 |
| 3.840 | 14 | 220 | 23.14 |
| 3.740 | 4 | 040 | 23.77 |
| 3.570 | 57 | 111 | 24.92 |
| 3.452 | 31 | 140 | 25.79 |
| 3.332 | 25 | 230 | 26.73 |
| 3.300 | 20 | 121 | 27.00 |
| 3.138 | 7 | 031 | 28.42 |
| 2.996 | 11 | 201 | 29.79 |
| 2.960 | 10 | 131 | 30.17 |
| 2.934 | 64 | 211 | 30.40 |
| 2.930 | | 310 | 30.48 |
| 2.871 | 18 | 240 | 31.12 |
| 2.839 | 31 | 150 | 31.48 |
| 2.782 | 100 | 221 | 32.15 |
| 2.775 | | 320 | 32.23 |
| 2.623 | 4 | 141 | 34.15 |
| 2.570 | 10 | 231 | 34.88 |
| 2.563 | | 330 | 34.98 |
| 2.491 | 4 | 250 | 36.03 |
| 2.404 | 48 | 051,160 | 37.38 |
| 2.371 | 6 | 311 | 37.91 |
| 2.336 | 15 | 340 | 38.51 |
| 2.287 | 11 | 321 | 39.37 |
| 2.214 | 2 | 410 | 40.71 |
| 2.181 | 2 | 260 | 41.37 |
| 2.164 | 6 | 331 | 41.71 |
| 2.146 | 2 | 420 | 42.06 |
| 2.115 | 3 | 350 | 42.71 |
| 2.081 | 3 | 170 | 43.44 |
| 2.066 | 8 | 161 | 43.77 |
| 2.044 | 12 | 430 | 44.28 |
| 2.021 | 48 | 341 | 44.80 |
| 2.017 | | 002 | 44.90 |
| 1.9580 | 13 | 401 | 46.33 |
| 1.9305 | 10 | 270 | 47.03 |
| 1.9178 | 9 | 261 | 47.36 |
| 1.9148 | 9 | 360 | 47.44 |
| 1.8941 | 5 | 421 | 47.99 |
| 1.8900 | | 071 | 48.10 |

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 1.8721 | 5 | 080,351 | 48.59 |
| 1.8496 | 14 | 171 | 49.22 |
| 1.8308 | 14 | 132 | 49.76 |
| 1.8235 | 16 | 431 | 49.97 |
| 1.7937 | 9 | 450 | 50.86 |
| 1.7790 | 2 | 510 | 51.31 |
| 1.7418 | 14 | 142,271,+ | 52.49 |
| 1.7387 | | 370 | 52.59 |
| 1.7296 | 6 | 361 | 52.89 |
| 1.7259 | 5 | 232 | 53.01 |
| 1.6684 | 4 | 181 | 54.99 |
| 1.6512 | 6 | 242 | 55.61 |
| 1.6455 | | 152 | 55.84 |
| 1.6395 | 4 | 451 | 56.04 |
| 1.6313 | 5 | 322 | 56.35 |
| 1.6163 | 2 | 540 | 56.92 |
| 1.6004 | 1 | 521 | 57.54 |
| 1.5679 | 1 | 252 | 58.85 |
| 1.5560 | 6 | 531 | 59.34 |
| 1.5454 | 5 | 162 | 59.79 |
| 1.5412 | 3 | 461 | 59.97 |
| 1.5264 | 3 | 342 | 60.61 |
| 1.5160 | 5 | 191 | 61.07 |
| 1.5005 | 5 | 541 | 61.77 |
| 1.4936 | 2 | 600 | 62.09 |
| 1.4642 | 5 | 620 | 63.48 |
| 1.4535 | 6 | 390 | 64.00 |
| 1.4363 | 7 | 480,551,+ | 64.86 |
| 1.3948 | 5 | 272,611 | 67.04 |
| 1.3871 | 3 | 1·10·1,640 | 67.46 |
| 1.3762 | 4 | 621 | 68.07 |
| 1.3726 | 4 | 082 | 68.27 |
| 1.3679 | 3 | 391 | 68.54 |
| 1.3534 | 3 | 481 | 69.38 |
| 1.3460 | 1 | 1·11·0 | 69.81 |
| 1.3402 | 5 | 452,2·10·1 | 70.16 |

## Reference

MacGillavry, C. H., Nijveld, H., Dierdorp, S., and Karsten, J. (1939). Die Krystallstruktur von $NH_4CdCl_3$ und $RbCdCl_3$, Rec. trav. chim., 58, 193-200.

Powder diffraction cards. None.

Additional published patterns. None.

**NBS sample.** The sample of rubidium cadmium trichloride was prepared at NBS by fusing rubidium chloride with anhydrous cadmium chloride at approximately 500° C.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of cesium and potassium, and 0.01 to 0.1 percent of sodium.

The sample was colorless. The crystals were optically uniaxial negative with very low double refraction, both indices being near 1.662.

$I/I_{corundum} = 4.5$.

**Structural data.** There is no published data on this form of rubidium cadmium trichloride. Its x-ray pattern is, however, very similar to cesium lead trichloride which has a tetragonal distorted perovskite structure. Rubidium cadmium trichloride has a superstructure requiring a double cell with 8 ($RbCdCl_3$) per cell.

This form is unstable at room temperature and inverts in a few days to the orthorhombic (low) form described by MacGillavry, Nijveld, Dierdorf, and Karsten (1939). Observations on a hot stage petrographic microscope show that the low form changes to the high form between 135° and 140° C. At about 190° C this form is seen to lose its double refraction, evidently changing to another high form, an undistorted cubic perovskite. This last change is rapidly reversible.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| NBS, sample at 25°C------ | 10.304 ± .001 | 10.399 ± .001 |

The density of rubidium cadmium trichloride, high form, calculated from the NBS lattice constants is 3.661 g/cm³ at 25° C.

Reference

MacGillavry, C.H., Nijveld, H., Dierdorf, S., and Karsten, J. (1939). Die Krystallstruktur von $NH_4CdCl_3$ und $RbCdCl_3$, Rec. Trav. Chim. 58, 193.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 5.196 | 14 | 002 | 17.05 |
| 5.152 | 18 | 200 | 17.20 |
| 3.655 | 100 | 202 | 24.33 |
| 3.262 | 4 | 301,310 | 27.32 |
| 3.111 | 2 | 311 | 28.67 |
| 2.985 | 10 | 222 | 29.91 |
| 2.761 | 2 | 312 | 32.40 |
| 2.599 | 28 | 004 | 34.48 |
| 2.550 | 46 | 400 | 34.81 |
| 2.321 | 6 | 204 | 38.77 |
| 2.305 | 9 | 420 | 39.05 |
| 2.116 | 24 | 224 | 42.69 |
| 2.107 | 35 | 422 | 42.88 |
| 1.830 | 25 | 404 | 49.79 |
| 1.822 | 8 | 440 | 50.01 |
| 1.724 | 5 | 424 | 53.07 |
| 1.720 | 2 | 442 | 53.22 |
| 1.6428 | 6 | 206 | 55.92 |
| 1.6295 | 8 | 602 | 56.42 |
| 1.4921 | 8 | 444 | 62.16 |
| 1.3850 | 8 | 426 | 67.59 |
| 1.3805 | 10 | 624 | 67.84 |
| 1.3778 | 4 | 642 | 68.00 |
| 1.2519 | 3 | 644 | 75.94 |
| 1.2496 | 2 | 802 | 76.11 |
| 1.2243 | 3 | 228 | 77.97 |
| 1.2203 | 3 | 606 | 78.28 |
| 1.2147 | 5 | 660,822 | 78.71 |
| 1.1603 | 3 | 408 | 83.19 |
| 1.1535 | 4 | 418 | 83.79 |
| 1.1513 | 3 | 840 | 83.98 |
| 1.1023 | 2 | 646 | 88.66 |
| 1.1004 | 3 | 664 | 88.85 |
| 1.0579 | 3 | 448 | 93.45 |
| 1.0531 | 2 | 844 | 94.01 |
| 1.0194 | 2 | 2·0·10 | 98.16 |
| 1.0161 | 3 | 628 | 98.59 |
| 1.0135 | 3 | 826 | 98.92 |
| 1.0107 | 4 | 862 | 99.30 |
| 0.9478 | 2 | 4·2·10 | 108.70 |

**Powder Diffraction File cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of rubidium manganese trifluoride was prepared at NBS by D. E. Roberts by heating rubidium fluoride and manganese difluoride to 1100°C.

Spectrographic analysis showed the following major impurities: <0.5 percent each of aluminum and silicon; 0.01 to 0.1 percent each of calcium, cesium, potassium, strontium, and vanadium.

The color of the sample was pale pink. The index of refraction is 1.483.

$I/I_{corundum} = 3.4$.

**Structural data.** Simanov, Batsanova, and Kovba (1957) determined that rubidium manganese trifluoride has the perovskite structure, the space group $O_h^1$-Pm3m (No. 221) and 1($RbMnF_3$) per unit cell.

*Lattice constants*

| | *a*(Å) |
|---|---|
| Simanova, Batsanova, and Kovba (1957) | 4.243 |
| Hoppe, Liebe, and Dähne (1961) | 4.25 |
| NBS, sample at 25°C | 4.2400 |

The density of rubidium manganese trifluoride calculated from the NBS lattice constant is 4.300 g/cm$^3$ at 25°C.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2$\theta$(°) |
|---|---|---|---|
| 4.235 | 2 | 100 | 20.96 |
| 2.998 | 100 | 110 | 29.78 |
| 2.447 | 20 | 111 | 36.70 |
| 2.119 | 50 | 200 | 42.63 |
| 1.895 | 2 | 210 | 47.97 |
| 1.731 | 32 | 211 | 52.85 |
| 1.499 | 21 | 220 | 61.85 |
| 1.413 | 2 | 300 | 66.05 |
| 1.341 | 19 | 310 | 70.13 |
| 1.278 | 9 | 311 | 74.11 |
| 1.2239 | 6 | 222 | 78.00 |
| 1.1759 | 2 | 320 | 81.84 |
| 1.1331 | 24 | 321 | 85.65 |
| 1.0599 | 4 | 400 | 93.22 |
| 1.0284 | 3 | 410 | 97.00 |
| 0.9993 | 7 | 411 | 100.85 |
| .9726 | 4 | 331 | 104.73 |
| .9481 | 17 | 420 | 108.67 |
| .9252 | 3 | 421 | 112.72 |
| .9040 | 4 | 332 | 116.86 |
| .8655 | 6 | 422 | 125.74 |
| .8315 | 14 | 510 | 135.74 |
| .8160 | 2 | 511 | 141.44 |

## References

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Simanov, Yu. P., Batsanova, L. P., and Kovba, L. M. (1957). X ray investigation of the binary fluorides of bivalent manganese, Russ. J. Inorg. Chem. 2, 207. (Translated from Zh. Neorgan. Khim. II, No. 10, 2410-2415.)

**Powder Diffraction File cards.** No. 14-38, Brown and McLaren (1962). Nos. 14-34 (cubic), 14-36 (cubic), and 14-37 (tetragonal) are for other forms of rubidium nitrate.

**Additional published patterns.** None.

**NBS sample.** The sample of rubidium nitrate was obtained from A.D. Mackay, Inc., New York, N.Y. The sample was recrystallized from aqueous solution at room temperature.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of potassium and sodium; 0.01 to 0.1 percent each of cesium and silicon.

The sample was colorless and optically positive with indices of refraction $N_e = 1.526$ and $N_o = 1.524$. A very slight 2V was noted.

**Structural data.** Pauling and Sherman (1933) proposed trigonal symmetry for rubidium nitrate, the probable space group $C_{3v}^2$-P31m (No. 157) and 9($RbNO_3$) per unit cell. Brown and McLaren (1962) reported that the space group was either $D_3^3$-$P3_112$ or $D_3^5$-$P3_212$.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Pauling and Sherman (1933) | 10.47 | 7.39 |
| Brown and McLaren (1962) | 10.48 | 7.45 |
| NBS, sample at 25°C | 10.479 | 7.452 |

The density of rubidium nitrate calculated from the NBS lattice constants is 3.109 g/cm$^3$ at 25°C.

Internal standard Ag, a = 4.08625 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2$\theta$(°) |
|---|---|---|---|
| 5.244 | <1 | 110 | 16.89 |
| 4.285 | 30 | 111 | 20.71 |
| 3.877 | <1 | 201 | 22.92 |
| 3.445 | 2 | 102 | 25.84 |
| 3.116 | 1 | 211 | 28.62 |
| 3.032 | 100 | 112 | 29.43 |
| 3.023 | 100 | 300 | 29.52 |
| 2.879 | 3 | 202 | 31.04 |
| 2.801 | 1 | 301 | 31.92 |
| 2.620 | 1 | 220 | 34.19 |
| 2.522 | 2 | 212,310 | 35.57 |
| 2.484 | 13 | 003 | 36.13 |
| 2.471 | 23 | 221 | 36.33 |
| 2.385 | 2 | 311 | 37.69 |
| 2.349 | 2 | 302 | 38.28 |
| 2.245 | 1 | 113 | 40.13 |
| 2.178 | 1 | 203 | 41.42 |
| 2.171 | 2 | 401 | 41.56 |
| 2.142 | 19 | 222 | 42.14 |
| 2.086 | 1 | 312 | 43.34 |
| 2.013 | 1 | 213 | 44.99 |
| 2.007 | 1 | 321 | 45.14 |
| 1.919 | 14 | 303 | 47.33 |
| 1.914 | 16 | 411 | 47.47 |
| 1.825 | 1 | 105 | 49.92 |
| 1.817 | 1 | 322 | 50.16 |
| 1.755 | 5 | 114 | 52.06 |
| 1.749 | 13 | 412 | 52.27 |
| 1.724 | <1 | 204 | 53.09 |
| 1.715 | 1 | 420 | 53.38 |
| 1.674 | 1 | 403 | 54.79 |
| 1.672 | 1 | 421 | 54.88 |
| 1.636 | 1 | 214 | 56.17 |
| 1.631 | 1 | 502,510 | 56.36 |
| 1.596 | 1 | 323 | 57.69 |
| 1.518 | 3 | 224 | 60.97 |
| 1.513 | 4 | 600 | 61.22 |
| 1.498 | 1 | 314 | 61.91 |
| 1.494 | 1 | 431 | 63.51 |
| 1.434 | 3 | 115 | 65.00 |

## References

Brown, R. N., and McLaren, A.C. (1962). The thermal transformation on solid rubidium nitrate, Acta Cryst. 15, 974-976.

Pauling, L., and Sherman, J. (1933). Note on the crystal structure of rubidium nitrate, Z. Krist. 84, 213-216.

| Internal standard Ag, a = 4.08625 Å<br>$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d* (Å) | *I* | *hkl* | 2θ(°) |
| 1.428 | 7 | 333 | 65.27 |
| 1.426 | | 521 | 65.37 |
| 1.416 | 1 | 205 | 65.88 |
| 1.412 | 1 | 423 | 66.11 |
| 1.3677 | 1 | 215 | 68.55 |
| 1.3570 | 5 | 414 | 69.17 |
| 1.3540 | 8 | 522 | 69.34 |
| 1.2955 | 2 | 225 | 72.96 |
| 1.2919 | 4 | 603 | 73.20 |
| 1.2770 | 1 | 701 | 74.19 |
| 1.2620 | 1 | 424 | 75.25 |
| 1.2356 | 1 | 442 | 77.13 |
| 1.1983 | 1 | 206 | 80.00 |
| 1.1909 | 1 | 415 | 80.60 |
| 1.1869 | 1 | 711 | 80.93 |
| 1.1676 | 1 | 216 | 82.55 |
| 1.1649 | 1 | 434 | 82.79 |
| 1.1491 | 2 | 703,306 | 84.18 |
| 1.1452 | 4 | 524 | 84.53 |
| 1.1436 | | 712 | 84.68 |
| 1.1226 | 1 | 623,226 | 86.65 |
| 1.1141 | 1 | 316 | 87.48 |
| 1.1113 | 1 | 614 | 87.75 |
| 1.0716 | 1 | 444 | 91.91 |

**Powder Diffraction File cards.** None.

**Additional published pattern.** Milligan, Watt, and Rachford (1949).

**NBS sample.** The sample of samarium vanadate was prepared at NBS. A mixture of samarium oxalate and vanadium pentoxide was heated at 850°C for 45 minutes.

Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, iron, magnesium, antimony, and silicon.

The color of the sample was strong yellow brown. The indices of refraction could not be determined because the sample was too fine-grained.

$I/I_{corundum} = 2.2$.

**Structural data.** Milligan, Watt, and Rachford (1949) determined that samarium vanadate has the zircon structure with the space group $D_{4h}^{19}$-$I4_1/amd$ (No. 141) and 4 ($SmVO_4$) per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Milligan, Watt, and Rachford (1949) | 7.22 | 6.35 |
| NBS, sample at 25°C | 7.2652 | 6.3894 |

The density of samarium vanadate calculated from the NBS lattice constants is 5.225 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 4.802 | 31 | 101 | 18.46 |
| 3.633 | 100 | 200 | 24.48 |
| 2.895 | 14 | 211 | 30.86 |
| 2.712 | 76 | 112 | 33.00 |
| 2.569 | 20 | 220 | 34.89 |
| 2.399 | 6 | 202 | 37.45 |
| 2.265 | 16 | 301 | 39.76 |
| 2.0438 | 9 | 103 | 44.28 |
| 1.9220 | 12 | 321 | 47.25 |
| 1.8653 | 56 | 312 | 48.78 |
| 1.8161 | 15 | 400 | 50.19 |
| 1.7810 | 6 | 213 | 51.25 |
| 1.6989 | 5 | 411 | 53.92 |
| 1.6244 | 11 | 420 | 56.61 |
| 1.5976 | 6 | 004 | 57.65 |
| 1.5096 | 14 | 332 | 61.36 |
| 1.4623 | 10 | 204 | 63.57 |
| 1.4171 | 4 | 501 | 65.85 |
| 1.3564 | 10 | 224 | 69.20 |
| 1.3011 | 11 | 512 | 72.60 |
| 1.2107 | 4 | 600 | 79.02 |
| 1.1996 | 6 | 404 | 79.89 |
| 1.1892 | 6 | 215 | 80.76 |
| 1.1607 | 7 | 532 | 83.15 |
| 1.1487 | 5 | 620 | 84.22 |
| 1.1389 | 11 | 424 | 85.11 |
| 1.0793 | 1 | 325 | 91.07 |
| 1.0425 | 7 | 116 | 95.27 |
| 1.0343 | 3 | 415 | 96.27 |
| 1.0074 | 3 | 640 | 99.74 |
| 0.9780 | 6 | 712 | 103.92 |
| .9660 | 8 | 316 | 105.76 |
| .9650 | 6 | 633,604 | 105.91 |
| .9327 | 6 | 624,703 | 111.24 |
| .9141 | 5 | 732 | 114.83 |
| .9040 | 4 | 723,336 | 116.88 |
| .8809 | 4 | 820 | 121.94 |
| .8787 | 4 | 217 | 122.46 |
| .8528 | 10 | 516,653 | 129.17 |
| .8166 | 4 | 752 | 141.22 |
| .8123 | 8 | 840 | 142.96 |
| .8095 | 10 | 536 | 144.16 |

## Reference

Milligan, W. O., Watt, L. M. and Rachford, H. H., Jr. (1949). X-ray & diffraction studies of heavy metal orthovanadates, J. Phys. & Colloid Chem. 53, 227-234.

**Powder Diffraction File cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of cubic silver antimony sulfide was prepared at NBS by heating miargyrite, $AgSbS_2$, in a closed tube at 600°C.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent silicon, and 0.01 to 0.1 percent each of aluminum, arsenic, bismuth, calcium, iron, germanium, magnesium, manganese, nickel, lead, and tungsten.

The sample was an opaque metallic gray powder.

$I/I_{corundum} = 3.5$.

**Structural data.** Geller and Wernick (1959) reported that high temperature silver antimony sulfide has the sodium chloride structure, the space group $O_h^5$-Fm3m (No. 225) and $2(AgSbS_2)$ per unit cell. Silver antimony sulfide also occurs as a natural mineral miargyrite which is monoclinic if formed below melting temperature of 450°C.

*Lattice constants*

| | *a(Å)* |
|---|---|
| Graham (1951) | 5.653 |
| Geller and Wernick (1959), sample at 25°C | 5.647 |
| NBS, sample at 25°C | 5.652 |

The density of cubic silver antimony sulfide calculated from the NBS lattice constant is 5.403 g/cm³ at 25°C.

Internal standard Ag, a = 4.08625 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d (Å)* | *I* | *hkl* | *2θ(°)* |
|---|---|---|---|
| 3.263 | 63 | 111 | 27.31 |
| 2.826 | 100 | 200 | 31.63 |
| 1.998 | 41 | 220 | 45.35 |
| 1.7039 | 21 | 311 | 53.75 |
| 1.6316 | 15 | 222 | 56.34 |
| 1.4131 | 7 | 400 | 66.06 |
| 1.2966 | 5 | 331 | 72.89 |
| 1.2635 | 7 | 420 | 75.12 |
| 1.1537 | 3 | 422 | 83.77 |
| 1.0877 | 3 | 511 | 90.17 |
| 0.9991 | 5 | 440 | 100.87 |
| .9553 | 2 | 531 | 107.47 |
| .9420 | 2 | 600 | 109.70 |
| .8936 | 1 | 620 | 119.08 |
| .8619 | 1 | 533 | 126.67 |
| .8520 | 1 | 622 | 129.39 |
| .8156 | <1 | 444 | 141.60 |
| .7913 | 2 | 711 | 153.53 |

## References

Geller, S. and Wernick, J. H. (1951). Ternary semiconducting compounds with sodium chloride-like structure: $AgSbSe_2$, $AgSbTe_2$, $AgBiS_2$, $AgBiSe_2$, Acta Cryst. 12, 46-54.

Graham, A. R. (1959). Matildite, aramayoite, miargyrite, Am. Mineralogist 36, 436-449.

**Powder Diffraction File cards.** No. 4-0675, Graham (1951).

**Additional published patterns.** Hofmann (1938).

**NBS sample.** The sample of miargyrite was obtained from Tem-pres Research Inc., State College, Pa.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent silicon, and 0.01 to 0.1 percent each of aluminum, arsenic, bismuth, calcium, iron, germanium, magnesium, manganese, nickel, lead, and tungsten.

The color of the sample was blackish red. The indices of refraction are very high and the sample was very fine-grained.

$I/I_{corundum} = 2.0$.

**Structural data.** Hofmann (1938) determined that miargyrite has the space group $C_{2h}^6$-A2/a (No. 15) and 8($AgSbS_2$) per unit cell. An irreversible cubic form is obtained at the melting point.

*Lattice constants*

| | *a*(Å) | *b* (Å) | *c*(Å) | *β*(°) |
|---|---|---|---|---|
| Hofmann (1938) | 13.20 | 4.40 | 12.86 | 98.06° |
| NBS, sample at 25°C | 13.224 | 4.410 | 12.881 | 98.48° |

The density of miargyrite calculated from the NBS lattice constants is 5.252 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2*θ*(°) |
|---|---|---|---|
| 4.259 | 4 | 202 | 20.84 |
| 3.440 | 81 | 211 | 25.88 |
| 3.186 | 31 | 004 | 27.98 |
| 3.101 | 30 | $\bar{4}02$ | 28.76 |
| 3.051 | 14 | $\bar{1}13$ | 29.25 |
| 2.892 | 100 | $\bar{2}13$ | 30.89 |
| 2.748 | 70 | 402 | 32.55 |
| 2.639 | 8 | $\bar{3}13$ | 33.94 |
| 2.265 | <1 | $\bar{5}11$ | 39.76 |
| 2.206 | 9 | 020 | 40.88 |
| 2.174 | 7 | 120 | 41.51 |
| 2.131 | 2 | 115 | 42.37 |
| 2.043 | 3 | 122 | 44.30 |
| 2.013 | 38 | $\bar{2}22$,215 | 44.99 |
| 1.971 | 27 | $\bar{6}11$ | 46.00 |
| 1.914 | 22 | $\bar{4}06$ | 47.45 |
| 1.875 | 5 | 315 | 48.51 |
| 1.871 | 4 | $\bar{6}13$ | 48.62 |
| 1.846 | 2 | 322 | 49.32 |
| 1.813 | 18 | 024 | 50.29 |
| 1.797 | 20 | $\bar{4}22$ | 50.77 |
| 1.737 | 4 | $\bar{7}11$ | 52.66 |
| 1.720 | 8 | 422 | 53.20 |
| 1.699 | 1 | $\bar{1}17$ | 53.93 |
| 1.693 | 12 | 613 | 54.14 |
| 1.686 | 14 | 520,$\bar{2}17$ | 54.38 |
| 1.672 | 7 | 406 | 54.88 |
| 1.660 | 8 | $\bar{6}15$ | 55.30 |
| 1.635 | 5 | 800 | 56.22 |
| 1.593 | 10 | 522,008 | 57.84 |
| 1.5504 | 9 | $\bar{8}04$,620 | 59.58 |
| 1.5301 | <1 | 802 | 60.45 |
| 1.5256 | <1 | $\bar{2}26$,$\bar{7}15$ | 60.65 |
| 1.4938 | 2 | $\bar{3}26$ | 62.08 |
| 1.4455 | 4 | $\bar{4}26$ | 64.40 |
| 1.4200 | 5 | 231,606 | 65.70 |
| 1.3990 | 1 | $\bar{8}06$ | 66.81 |
| 1.3873 | 2 | $\bar{6}08$ | 67.45 |
| 1.3860 | 2 | $\bar{5}26$ | 67.52 |
| 1.3747 | 6 | 804 | 68.15 |
| 1.3321 | 6 | 426 | 70.65 |
| 1.3135 | 5 | 820 | 71.81 |
| 1.2850 | 5 | 219 | 73.65 |
| 1.2731 | <1 | $\bar{5}19$ | 74.46 |
| 1.2683 | 4 | $\bar{8}24$ | 74.79 |

## References

Graham, A. R. (1951). Matildite, aramayoite, miargyrite, Am. Mineralogist 36, 436-449.

Hofmann, W. (1938). Die Struktur von Miargyrit, $AgSbS_2$, Sitzber. preuss. Akad Wiss. Physik. Math. Kl. Berlin 7, 111-119.

| Internal standard W, a = 3.16504 Å<br>$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d* (Å) | *I* | *hkl* | 2θ(°) |
| 1.2583 | 1 | 135 | 75.49 |
| 1.2520 | 6 | $\bar{5}33, \bar{1}0\cdot1\cdot3$ | 75.93 |
| 1.2314 | 5 | 10·1·1 | 77.44 |
| 1.2261 | 5 | $\bar{6}19$ | 77.84 |
| 1.1833 | 1 | $\bar{9}24$ | 81.22 |
| 1.1734 | 1 | 717 | 82.05 |
| 1.1663 | 2 | 824 | 82.66 |
| 1.1462 | 3 | $\bar{6}33$ | 84.44 |
| 1.1446 | 3 | $\bar{2}37$ | 84.59 |
| 1.1361 | 1 | $\bar{6}35$ | 85.37 |
| 1.1316 | 4 | $4\cdot0\cdot10, \bar{2}\cdot1\cdot11$ | 85.79 |
| 1.1084 | 2 | $1\bar{0}\cdot1\cdot7$ | 88.04 |
| 1.1016 | 1 | $\bar{1}2\cdot0\cdot2$ | 88.73 |
| 1.0894 | 2 | 733 | 89.99 |
| 1.0877 | 3 | $1\cdot2\cdot10, \bar{5}\cdot1\cdot11$ | 90.17 |
| 1.0784 | 1 | 2·1·11 | 91.16 |
| 1.0777 | 2 | $\bar{8}28$ | 91.24 |
| 1.0669 | 2 | $10\cdot1\cdot5, \bar{1}2\cdot1\cdot1$ | 92.43 |
| 1.0648 | <1 | 808 | 92.67 |
| 1.0619 | <1 | 826, 0·0·12 | 93.00 |
| 1.0491 | 1 | 437, 3·1·11, + | 94.48 |
| 1.0466 | 1 | 10·0·6, 11·2·0 | 94.77 |
| 1.0421 | 2 | $\bar{8}35, \bar{1}44, 12\cdot1\cdot1$ | 95.32 |
| 1.0392 | 2 | $\bar{6}\cdot2\cdot10$ | 95.67 |
| 1.0355 | 1 | 6·0·10 | 96.12 |
| 1.0239 | <1 | $\bar{2}39, 2\cdot0\cdot12$ | 97.57 |
| 1.0135 | 2 | 537 | 98.92 |
| 1.0077 | 2 | $\bar{7}\cdot2\cdot10$ | 99.71 |
| 0.9917 | <1 | 239 | 101.91 |
| .9855 | 1 | $\bar{1}2\cdot2\cdot2$ | 102.81 |
| .9801 | <1 | 5·1·11 | 103.60 |
| .9762 | 2 | $1\bar{0}\cdot3\cdot3, \bar{6}37$ | 104.19 |
| .9748 | <1 | 819 | 104.40 |
| .9708 | 1 | $\bar{1}2\cdot2\cdot4, 146$ | 105.02 |
| .9661 | <1 | $10\cdot3\cdot1, \bar{1}3\cdot0\cdot6$ | 105.74 |
| .9637 | 1 | $\bar{3}\cdot1\cdot13, \bar{6}39$ | 106.11 |
| .9590 | 1 | 828 | 106.86 |
| .9570 | 2 | $\bar{8}\cdot0\cdot12$ | 107.20 |
| .9475 | <1 | $1\bar{0}\cdot3\cdot5, 12\cdot2\cdot2$ | 108.76 |
| .9452 | <1 | 10·2·6, 439 | 109.16 |
| .9435 | 2 | $\bar{5}\cdot1\cdot13, 6\cdot1\cdot11$ | 109.45 |

**Powder Diffraction File cards.** No. 14-280, Toulmin (1963).

**Additional published patterns.** None.

**NBS sample.** The sample of pyrargyrite was obtained from Tem-pres Research Inc., State College, Pa. It was annealed at 350°C over night in order to sharpen the diffraction pattern.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum, arsenic, iron, germanium, molybdenum, lead, silicon, strontium, and tungsten.

The color of the sample was gray reddish brown. The indices of refraction are very high and the sample was very fine-grained.

$I/I_{corundum} = 1.1$.

**Structural data.** Grossner and Mussgnug (1928) determined that pyrargyrite is isostructural with proustite with the space group $C_{3v}^6$-R3c (No. 161), and $6(Ag_3SbS_3)$ per unit cell.

The unit cell measurements reported by Grossner and Mussgnug were converted from rhombohedral kX units to hexagonal angstrom units.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Grossner and Mussgnug (1928) | 11.14 | 8.79 |
| Hocart (1937) | 11.05 | 8.74 |
| Toulmin (1963) | 11.052 | 8.7177 |
| NBS, sample at 25°C | 11.047 | 8.719 |

The density of pyrargyrite calculated from the NBS lattice constants is 5.855 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 3.962 | 15 | 012 | 22.42 |
| 3.338 | 53 | 211 | 26.68 |
| 3.220 | 67 | 202 | 27.68 |
| 3.185 | 57 | 300 | 27.99 |
| 2.780 | 100 | 122 | 32.17 |
| 2.761 | 9 | 220 | 32.40 |
| 2.571 | 60 | 113 | 34.86 |
| 2.538 | 60 | 131 | 35.34 |
| 2.267 | 19 | 312 | 39.73 |
| 2.128 | 20 | 321 | 42.43 |
| 2.096 | 7 | 042 | 43.11 |
| 2.088 | 10 | 410 | 43.30 |
| 2.002 | 3 | 223 | 45.26 |
| 1.983 | 5 | 024 | 45.72 |
| 1.961 | 29 | 232 | 46.26 |
| 1.867 | 22 | 214 | 48.73 |
| 1.842 | 8 | 330 | 49.44 |
| 1.771 | 8 | 241 | 51.56 |
| 1.7521 | 16 | 502 | 52.16 |
| 1.6957 | 8 | 413 | 54.03 |
| 1.6842 | 19 | 134 | 54.43 |
| 1.6703 | 14 | 422 | 54.92 |
| 1.6111 | 9 | 404 | 57.12 |
| 1.5983 | 11 | 152 | 57.62 |
| 1.5943 | | 600 | 57.78 |
| 1.5703 | 4 | 125 | 58.75 |
| 1.5553 | 3 | 333 | 59.37 |
| 1.5480 | 4 | 431 | 59.68 |
| 1.5322 | 10 | 520 | 60.36 |
| 1.4796 | 2 | 342 | 62.74 |
| 1.4576 | 8 | 315 | 63.80 |
| 1.4535 | | 006 | 64.00 |
| 1.4389 | 2 | 161 | 64.73 |
| 1.4052 | 5 | 116 | 66.48 |
| 1.3915 | 8 | 244 | 67.22 |
| 1.3835 | 4 | 612 | 67.66 |
| 1.3654 | 2 | 235 | 68.68 |
| 1.3554 | 5 | 523 | 69.26 |
| 1.3495 | 6 | 514 | 69.61 |
| 1.3225 | 1 | 306 | 71.24 |
| 1.3114 | 1 | 621 | 71.94 |
| 1.3040 | 1 | 532 | 72.41 |
| 1.2861 | 3 | 226 | 73.58 |
| 1.2752 | 1 | 434 | 74.32 |
| 1.2693 | <1 | 262 | 74.72 |

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Grossner, B. and Mussgnug, F. (1928). Original-Mitteilungen an die Redaktion. Über die Kristallstruktur von Pyrargyrit, Centr. Mineral., Geol. 65-73.

Hocart, R. (1937). Schéma structurale de la proustite et de la pyrargyrite, Compt. rend. **205**, 68-70.

Toulmin, P., 3rd. (1963). Proustite-pyrargyrite solid solutions, Am. Mineralogist **48**, Nos. 7 & 8, 725-736.

| Internal standard W, a = 3.16504 Å<br>CuK$\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C | | | |
|---|---|---|---|
| *d* (Å) | *I* | *hkl* | 2$\theta$(°) |
| 1.2672 | 2 | 710 | 74.87 |
| 1.2551 | <1 | 425 | 75.71 |
| 1.2128 | 4 | 164 | 78.88 |
| 1.2053 | <1 | 630,027 | 79.43 |
| 1.1926 | 4 | 416 | 80.46 |
| 1.1793 | 4 | 452 | 81.56 |
| 1.1682 | <1 | 345 | 82.50 |
| 1.1614 | 2 | 713 | 83.09 |
| 1.1580 | 4 | 271,704 | 83.39 |
| 1.1533 | 1 | 802 | 83.81 |
| 1.1406 | 3 | 336 | 84.95 |
| 1.1334 | 3 | 624 | 85.62 |
| 1.1275 | 1 | 137 | 86.18 |
| 1.1046 | 2 | 550,407 | 88.42 |
| 1.0849 | 1 | 182 | 90.47 |
| 1.0831 | 2 | 327,018 | 90.66 |
| 1.0758 | 1 | 535 | 91.45 |
| 1.0742 | 2 | 606 | 91.62 |
| 1.0681 | 3 | 731,544 | 92.30 |
| 1.0633 | 1 | 900 | 92.83 |
| 1.0451 | 2 | 372 | 94.96 |
| 1.0439 | 1 | 820,057 | 95.10 |
| 1.0302 | 1 | 274 | 96.77 |
| 1.0088 | <1 | 517 | 99.55 |
| 0.9962 | 2 | 191 | 101.28 |
| .9764 | 3 | 437 | 104.16 |
| .9652 | 1 | 381,734 | 105.88 |
| .9552 | 4 | 716 | 107.48 |
| .9485 | 1 | 832 | 108.60 |
| .9474 | 1 | 167 | 108.77 |

**Powder Diffraction File cards.** No. 3-0707, Terrey and Diamond (1928).

**Additional published patterns.** None.

**NBS sample.** The sample of silver subfluoride was supplied by L. D. Calvert of the Division of Applied Chemistry, National Research Council, Canada. It was prepared in that Division by P. Tymchuk by reacting pure silver with hydrogen fluoride and 30% hydrogen peroxide. A uniform precipitate was obtained when the sample was washed with alcohol and ether.

Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, copper, iron, magnesium, silicon, and tin.

The sample has a metallic luster and it was a light olive opaque powder.

$I/I_{corundum} = 3.2$.

**Structural data.** Ott and Seyfarth (1928) determined that silver subfluoride has the cadmium iodide structure, the space group $D^3_{3d}$-$P\bar{3}ml$ (No. 164) and $1(Ag_2F)$ per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Terrey and Diamond (1928) | 2.995 | 5.722 |
| Ott and Seyfarth (1928) | 3.0 | 5.75 |
| NBS, sample at 25°C | 3.0016 | 5.7014 |

The density of silver subfluoride calculated from the NBS lattice constants is 8.762 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 5.701 | 16 | 001 | 15.53 |
| 2.849 | 28 | 002 | 31.37 |
| 2.600 | 16 | 100 | 34.47 |
| 2.365 | 100 | 101 | 38.01 |
| 1.921 | 27 | 102 | 47.27 |
| 1.9000 | 16 | 003 | 47.83 |
| 1.5340 | 8 | 103 | 60.28 |
| 1.5010 | 11 | 110 | 61.75 |
| 1.4515 | 4 | 111 | 64.10 |
| 1.4248 | 4 | 004 | 65.45 |
| 1.3280 | 5 | 112 | 70.90 |
| 1.2999 | 2 | 200 | 72.67 |
| 1.2673 | 7 | 201 | 74.86 |
| 1.2499 | 8 | 104 | 76.09 |
| 1.1825 | 4 | 202 | 81.29 |
| 1.1777 | 6 | 113 | 81.69 |
| 1.1403 | 2 | 005 | 84.98 |
| 1.0729 | 1 | 203 | 91.77 |
| 1.0444 | 4 | 105 | 95.04 |
| 1.0334 | 2 | 114 | 96.38 |
| 0.9824 | 2 | 210 | 103.26 |
| .9682 | 5 | 211 | 105.41 |
| .9605 | 3 | 204 | 106.63 |
| .9502 | 1 | 006 | 108.31 |
| .9290 | 2 | 212 | 112.02 |
| .9080 | 4 | 115 | 116.05 |
| .8926 | 4 | 106 | 119.30 |
| .8727 | 1 | 213 | 123.91 |
| .8665 | 2 | 300 | 125.47 |
| .8572 | 1 | 205,301 | 127.94 |
| .8289 | 2 | 302 | 136.62 |
| .8148 | 3 | 007 | 141.92 |
| .8089 | 2 | 214 | 144.42 |
| .8029 | 1 | 116 | 147.21 |
| .7884 | 1 | 303 | 155.38 |

## References

Ott, H. and Seyfarth, H. (1928). Die Struktur des Silbersubfluoride, Z. Krist. 67, 430-433.

Terrey, H. and Diamond, H. (1928). The crystal structure of silver subfluoride, J. Chem. Soc. (London), 2820-2824.

**Powder Diffraction File cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of sodium hexametaphosphate hexahydrate was prepared by E. J. Griffith (1965) of the Inorganic Chemicals Division, Monsanto Co., St. Louis, Mo.

Spectrographic analysis showed the following major impurities: 0.001 to 0.1 percent each of aluminum and silicon.

The sample is colorless and optically positive. The indices of refraction are $N_\alpha = 1.458 \pm .001$, $N_\beta = 1.453 \pm .001$, and $N_\gamma = 1.459 \pm .001$. 2V is large.

$I/I_{corundum} = 0.8$.

**Structural data.** Jost (1965) determined that sodium hexametaphosphate hexahydrate has the space group $D_{2h}^{18}$-Ccmb (No. 64) or $C_{2v}^{17}$-Cc2b (No. 41) and $4(Na_6P_6O_{18}\cdot 6H_2O)$ per unit cell.

*Lattice constants*

| | *a*(Å) | *b*(Å) | *c*(Å) |
|---|---|---|---|
| Jost (1965) | 11.58 | 18.54 | 10.48 |
| NBS, sample at 25°C | 11.547 | 18.492 | 10.495 |

The density of sodium hexametaphosphate hexahydrate calculated from the NBS lattice constants is 2.134 g/cm³ at 25°C.

Internal standard Ag, a = 4.08625 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 9.24 | 18 | 020 | 9.56 |
| 7.17 | 100 | 111 | 12.34 |
| 5.245 | 42 | 002 | 16.89 |
| 5.058 | 77 | 201 | 17.52 |
| 4.900 | 76 | 220 | 18.09 |
| 4.831 | 47 | 131 | 18.35 |
| 4.626 | 28 | 112,040 | 19.17 |
| 4.567 | 24 | 022 | 19.42 |
| 3.885 | 3 | 202 | 22.87 |
| 3.776 | 3 | 132 | 23.54 |
| 3.583 | 88 | 222 | 24.83 |
| 3.546 | 28 | 311 | 25.09 |
| 3.467 | 14 | 042 | 25.67 |
| 3.338 | 15 | 151 | 26.68 |
| 3.292 | 73 | 113 | 27.06 |
| 3.117 | 30 | 331 | 28.61 |
| 3.083 | 15 | 060 | 28.94 |
| 3.060 | 4 | 312 | 29.16 |
| 2.974 | 11 | 242 | 30.02 |
| 2.942 | 15 | 133 | 30.36 |
| 2.926 | 13 | 152 | 30.53 |
| 2.888 | 2 | 400 | 30.94 |
| 2.783 | 4 | 401 | 32.14 |
| 2.755 | 6 | 420 | 32.47 |
| 2.719 | 18 | 260 | 32.91 |
| 2.664 | 19 | 421 | 33.61 |
| 2.632 | 14 | 261 | 34.04 |
| 2.623 | 6 | 004 | 34.15 |
| 2.584 | 26 | 351 | 34.68 |
| 2.529 | 5 | 402 | 35.46 |
| 2.482 | <2 | 153 | 36.16 |
| 2.440 | 5 | 422 | 36.81 |
| 2.414 | 18 | 262 | 37.21 |
| 2.386 | 27 | 441,333 | 37.67 |
| 2.312 | 15 | 224,172,080 | 38.92 |
| 2.238 | 4 | 511 | 40.26 |
| 2.227 | 3 | 403 | 40.47 |
| 2.164 | 5 | 423 | 41.70 |
| 2.147 | 14 | 263 | 42.05 |
| 2.121 | 11 | 353 | 42.59 |
| 2.104 | 18 | 154 | 42.94 |
| 2.073 | 7 | 173 | 43.63 |
| 2.067 | 5 | 461 | 43.76 |
| 2.012 | 8 | 372 | 45.02 |
| 2.006 | 6 | 443 | 45.15 |
| 1.972 | 2 | 205 | 45.98 |
| 1.955 | 4 | 462 | 46.41 |
| 1.925 | 4 | 551,600 | 47.17 |
| 1.917 | 2 | 513 | 47.38 |
| 1.893 | 11 | 601 | 48.02 |

## References

Griffth, E. J. and Buxton, R. L. (1965). The preparation and properties of the twelve-membered ring hexametaphosphate anion, Inorg. Chem. 4, 549.

Jost, K-H. (1965). Die Struktur des Natrium-hexametaphosphates $Na_6(P_6O_{18}).6H_2O$. Acta Cryst. 19, 555-560.

Internal standard Ag, a = 4.08625 Å
$CuK\alpha_1$ λ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 1.888 | 9 | 264,192 | 48.16 |
| 1.871 | 6 | 354 | 48.63 |
| 1.850 | 4 | 0·10·0,373 | 49.22 |
| 1.835 | 3 | 552 | 49.64 |
| 1.829 | 2 | 283 | 49.81 |
| 1.806 | 4 | 602,463 | 50.50 |
| 1.765 | 2 | 335 | 51.74 |
| 1.748 | 4 | 006 | 52.28 |
| 1.734 | <2 | 084 | 52.74 |
| 1.726 | 3 | 514 | 53.02 |
| 1.715 | 4 | 571 | 53.38 |
| 1.707 | 3 | 482 | 53.66 |
| 1.686 | 3 | 603 | 54.36 |
| 1.669 | 2 | 425,2·10·2,534 | 54.97 |
| 1.661 | 2 | 265,284 | 55.24 |
| 1.649 | 4 | 355 | 55.71 |
| 1.632 | <2 | 660 | 56.31 |
| 1.613 | <2 | 661 | 57.05 |
| 1.609 | <2 | 393 | 57.20 |
| 1.601 | <2 | 194 | 57.50 |
| 1.587 | <2 | 316,1·11·2 | 58.08 |
| 1.567 | 4 | 712,156 | 58.87 |
| 1.5568 | 3 | 4·10·0,573 | 59.31 |
| 1.5520 | 4 | 604 | 59.51 |
| 1.5475 | 4 | 515 | 59.70 |
| 1.5414 | 4 | 336,0·12·0 | 59.96 |
| 1.5192 | 2 | 591 | 60.93 |
| 1.5109 | 3 | 0·10·4,375 | 61.30 |
| 1.5065 | 4 | 750,535 | 61.50 |
| 1.5025 | 4 | 1·11·3 | 61.68 |
| 1.4869 | <2 | 465,713,484 | 62.40 |
| 1.4794 | 3 | 663,680,027 | 62.75 |
| 1.4744 | 3 | 2·12·1 | 62.99 |
| 1.4706 | <2 | 266,644 | 63.17 |
| 1.4560 | 2 | 195 | 63.88 |
| 1.4330 | <2 | 227,2·12·2 | 65.03 |
| 1.4256 | <2 | 820 | 65.41 |
| 1.4234 | <2 | 682,446 | 65.52 |
| 1.4131 | <2 | 821 | 66.06 |
| 1.4058 | <2 | 593 | 66.45 |
| 1.4024 | <2 | 625 | 66.63 |
| 1.3944 | 2 | 086 | 67.06 |
| 1.3919 | 2 | 802 | 67.20 |
| 1.3837 | 2 | 753 | 67.65 |
| 1.3799 | <2 | 157 | 67.86 |
| 1.3760 | <2 | 822 | 68.08 |
| 1.3561 | <2 | 645,286 | 69.22 |
| 1.3483 | <2 | 4·12·1,5·11·1 | 69.68 |
| 1.3303 | 3 | 407 | 70.76 |
| 1.3238 | <2 | 3·13·1 | 71.16 |

**Powder Diffraction File cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of terbium vanadate was prepared at NBS. A mixture of terbium oxalate and vanadium pentoxide was heated 1 hr. at 1400°C.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of aluminum, iron, and lead.

The color of the sample was gray yellow. The indices of refraction could not be determined because the sample was to fine-grained.

$I/I_{corundum} = 2.6$.

**Structural data.** Milligan, Watt, and Rachford (1949) determined that terbium vanadate is isostructural with zircon with the space group $D_{4h}^{19}$ - $I4_1/amd$ (No. 141) and $4(TbVO_4)$ per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Milligan and Vernon (1952) | 7.15 | 6.31 |
| NBS, sample at 25°C | 7.1772 | 6.3289 |

The density of terbium vanadate calculated from the NBS lattice constants is 5.579 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 4.75 | 33 | 101 | 18.66 |
| 3.587 | 100 | 200 | 24.80 |
| 2.862 | 12 | 211 | 31.22 |
| 2.684 | 76 | 112 | 33.35 |
| 2.537 | 22 | 220 | 35.35 |
| 2.374 | 4 | 202 | 37.87 |
| 2.238 | 17 | 301 | 40.26 |
| 2.024 | 11 | 103 | 44.73 |
| 1.899 | 11 | 321 | 47.86 |
| 1.844 | 60 | 312 | 49.38 |
| 1.794 | 16 | 400 | 50.85 |
| 1.763 | 6 | 213 | 51.81 |
| 1.679 | 5 | 411 | 54.61 |
| 1.606 | 12 | 420 | 57.34 |
| 1.5823 | 7 | 303,004 | 58.26 |
| 1.4914 | 18 | 332 | 62.19 |
| 1.4471 | 14 | 323,204 | 64.32 |
| 1.3996 | 6 | 501 | 66.78 |
| 1.3422 | 11 | 413,224 | 70.04 |
| 1.2858 | 10 | 512 | 73.60 |
| 1.2686 | 4 | 440 | 74.77 |
| 1.1960 | 4 | 600 | 80.19 |
| 1.1862 | 8 | 404,503 | 80.98 |
| 1.1770 | 3 | 215 | 81.75 |
| 1.1597 | 2 | 611 | 83.24 |
| 1.1470 | 8 | 532 | 84.37 |
| 1.1345 | 5 | 620 | 85.52 |
| 1.1262 | 10 | 424,523 | 86.30 |
| 1.1034 | 2 | 541 | 88.54 |
| 1.0681 | 4 | 325,622 | 92.30 |
| 1.0322 | 5 | 116 | 96.53 |
| 1.0296 | 4 | 613 | 96.85 |
| 1.0234 | 2 | 415 | 97.64 |
| 0.9956 | 4 | 640 | 101.36 |
| .9898 | 4 | 543,444 | 102.19 |
| .9666 | 8 | 712 | 105.67 |
| .9562 | 4 | 316 | 107.32 |
| .9540 | 6 | 633,604 | 107.69 |
| .9220 | 6 | 703,624 | 113.31 |
| .9031 | 6 | 732 | 117.05 |
| .8971 | 3 | 800,107 | 118.31 |
| .8948 | 4 | 336 | 118.81 |
| .8702 | 4 | 820,217 | 124.54 |
| .8438 | 6 | 516 | 131.81 |
| .8067 | 6 | 752 | 145.43 |
| .8007 | 6 | 536 | 148.31 |

## References

Milligan, W. O., and Vernon, L. W. (1952). Crystal structure of heavy metal orthovanadates, J. Phys. Chem. 56, 145.

Milligan, W. O., Watt, L. M., and Rachford, H. H., Jr. (1949). X-ray diffraction studies on heavy metal orthovanadates, J. Phys. and Colloid Chem. 53, 227-234.

## Thulium Vanadate, $TmVO_4$ (tetragonal)

**Powder Diffraction File cards.** None.

**Additional published patterns.** Milligan, Watt, and Rachford (1949).

**NBS sample.** The sample of thulium vanadate was prepared at NBS. A mixture of thulium oxalate and vanadium pentoxide was heated at 1400°C for 1 hr.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum and silicon, and 0.001 to 0.01 percent magnesium.

The color of the sample was dark gray yellow. The indices of refraction could not be determined because the sample was too fine-grained.

$I/I_{corundum} = 3.6$.

**Structural data.** Milligan, Watt, and Rachford (1949) determined that thulium vanadate has the zircon structure with the space group $D_{4h}^{19}$-$I4_1/amd$ (No. 141) and 4($TmVO_4$) per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Milligan, Watt, and Rachford (1949) | 7.00 | 6.21 |
| NBS, sample at 25°C | 7.0712 | 6.2606 |

The density of thulium vanadate calculated from the NBS lattice constants is 6.023 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 4.686 | 33 | 101 | 18.92 |
| 3.535 | 100 | 200 | 25.17 |
| 2.824 | 12 | 211 | 31.66 |
| 2.654 | 68 | 112 | 33.74 |
| 2.500 | 19 | 220 | 35.89 |
| 2.344 | 3 | 202 | 38.36 |
| 2.2061 | 16 | 301 | 40.87 |
| 2.0014 | 2 | 103 | 45.27 |
| 1.8714 | 11 | 321 | 48.61 |
| 1.8192 | 52 | 312 | 50.10 |
| 1.7678 | 22 | 400 | 51.66 |
| 1.7421 | 5 | 213 | 52.48 |
| 1.6543 | 3 | 411 | 55.50 |
| 1.5816 | 10 | 420 | 58.29 |
| 1.5652 | 5 | 004 | 58.96 |
| 1.5626 | 4 | 303 | 59.07 |
| 1.4710 | 12 | 332 | 63.15 |
| 1.4310 | 10 | 204 | 65.13 |
| 1.3790 | 4 | 501 | 67.91 |
| 1.3261 | 8 | 224 | 71.02 |
| 1.2850 | <1 | 521 | 73.65 |
| 1.2678 | 10 | 512 | 74.83 |
| 1.2498 | 4 | 440 | 76.09 |
| 1.1784 | 4 | 600 | 81.63 |
| 1.1716 | 5 | 404 | 82.21 |
| 1.1643 | 2 | 215 | 82.84 |
| 1.1428 | 2 | 611 | 84.75 |
| 1.1306 | 6 | 532 | 85.89 |
| 1.1181 | 4 | 620 | 87.08 |
| 1.1121 | 8 | 424 | 87.67 |
| 1.0550 | 2 | 325 | 93.79 |
| 1.0392 | 2 | 631 | 95.67 |
| 1.0214 | 3 | 116 | 97.89 |
| 1.0156 | 2 | 613 | 98.65 |
| 0.9805 | 4 | 640 | 103.54 |
| .9765 | 4 | 444,543 | 104.15 |
| .9524 | 8 | 712 | 107.95 |
| .9454 | 6 | 316 | 109.13 |
| .9412 | 4 | 604,633 | 109.84 |
| .9097 | 5 | 624,703 | 115.72 |
| .9063 | 4 | 525 | 116.39 |
| .8901 | 4 | 732 | 119.85 |
| .8841 | 3 | 336,800 | 121.20 |
| .8685 | 2 | 811 | 124.96 |
| .8606 | 2 | 217 | 127.03 |
| .8574 | 3 | 820 | 127.88 |
| .8337 | 8 | 660,516 | 135.00 |
| .8309 | 6 | 644 | 135.94 |
| .8307 | 4 | 653 | 136.00 |
| .8084 | 1 | 813 | 144.65 |
| .7949 | 4 | 752 | 151.38 |
| .7908 | 4 | 536,840 | 153.82 |

### Reference

Milligan, W. O., Watt, L. M., and Rachford, H. H., Jr. (1949). X-ray diffraction studies of heavy metal orthovanadates, J. Phys. and Colloid Chem. 53, 227-234.

**Powder Diffraction File cards.** None.

**Additional published patterns.** Milligan, Watt, and Rachford (1949).

**NBS sample.** The sample of ytterbium vanadate was prepared at NBS. A mixture of ytterbium oxalate and vanadium pentoxide was heated at 1400°C for 1 hr.

Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum and silicon, and 0.001 to 0.01 percent each of calcium, iron, and magnesium.

The color of the sample was dark gray yellow. The indices of refraction could not be determined because the sample was too fine-grained.

$I/I_{corundum} = 3.7$.

**Structural data.** Milligan, Watt, and Rachford (1949) determined that ytterbium vanadate is isostructural with zircon with the space group $D_{4h}^{19}$-$I4_1/amd$ (No. 141) and $4(YbVO_4)$ per unit cell.

*Lattice constants*

| | a(Å) | c(Å) |
|---|---|---|
| Milligan, Watt, and Rachford (1949) | 7.02 | 6.23 |
| NBS, sample at 25°C | 7.0435 | 6.2470 |

The density of ytterbium vanadate calculated from the NBS lattice constants is 6.172 g/cm³ at 25°C.

## Reference

Milligan, W. O., Watt, L. M., and Rachford, H. H., Jr. (1949). X-ray diffraction studies of heavy metal orthovanadates, J. Phys. and Colloid Chem. 53, 227-234.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| d (Å) | I | hkl | 2θ(°) |
|---|---|---|---|
| 4.674 | 47 | 101 | 18.97 |
| 3.523 | 100 | 200 | 25.26 |
| 2.813 | 15 | 211 | 31.78 |
| 2.646 | 77 | 112 | 33.85 |
| 2.491 | 25 | 220 | 36.03 |
| 2.337 | 4 | 202 | 38.47 |
| 2.1979 | 20 | 301 | 41.03 |
| 1.9972 | 12 | 103 | 45.37 |
| 1.8649 | 16 | 321 | 48.79 |
| 1.8137 | 61 | 312 | 50.26 |

continued

| d (Å) | I | hkl | 2θ(°) |
|---|---|---|---|
| 1.7609 | 18 | 400 | 51.88 |
| 1.7372 | 6 | 213 | 52.64 |
| 1.6477 | 6 | 411 | 55.74 |
| 1.5752 | 13 | 420 | 58.55 |
| 1.5620 | 6 | 004 | 59.09 |
| 1.5575 | 7 | 303 | 59.28 |
| 1.4662 | 16 | 332 | 63.38 |
| 1.4273 | 12 | 204 | 65.32 |
| 1.3739 | 6 | 501 | 68.20 |
| 1.3227 | 10 | 224 | 71.23 |
| 1.3203 | 4 | 413 | 71.38 |
| 1.2800 | 2 | 521 | 73.99 |
| 1.2632 | 11 | 512 | 75.15 |
| 1.2450 | 3 | 440 | 76.44 |
| 1.1736 | 4 | 600 | 82.04 |
| 1.1681 | 6 | 404 | 82.51 |
| 1.1612 | 3 | 215 | 83.11 |
| 1.1385 | 2 | 611 | 85.15 |
| 1.1265 | 10 | 532 | 86.28 |
| 1.1136 | 5 | 620 | 87.53 |
| 1.1088 | 11 | 424 | 88.00 |
| 1.0834 | 1 | 541 | 90.63 |
| 1.0524 | 2 | 325 | 94.09 |
| 1.0354 | 2 | 631 | 96.13 |
| 1.0191 | 4 | 116 | 98.19 |
| 1.0120 | 2 | 613 | 99.13 |
| 1.0085 | 1 | 415 | 99.59 |
| 0.9932 | 1 | 701 | 101.70 |
| .9767 | 4 | 640 | 104.12 |
| .9736 | 4 | 444 | 104.58 |
| .9560 | 1 | 721 | 107.36 |
| .9490 | 8 | 712 | 108.52 |
| .9432 | 6 | 316 | 109.50 |
| .9384 | 4 | 604 | 110.34 |
| .9348 | 2 | 505 | 110.97 |
| .9067 | 6 | 624 | 116.32 |
| .9034 | 3 | 525 | 116.99 |
| .8867 | 6 | 732 | 120.60 |
| .8820 | 3 | 336 | 121.68 |
| .8652 | 2 | 811 | 125.81 |
| .8586 | 2 | 217 | 127.56 |
| .8542 | 2 | 820 | 128.78 |
| .8492 | 1 | 615 | 130.19 |
| .8315 | 7 | 516 | 135.75 |
| .8281 | 6 | 644 | 136.92 |
| .8174 | 1 | 831 | 140.87 |
| .8117 | 1 | 327 | 143.22 |
| .8056 | 2 | 813 | 145.91 |
| .8037 | 2 | 635 | 146.81 |
| .7920 | 4 | 752 | 153.05 |

## Yttrium Vanadate, $YVO_4$ (tetragonal)

**Powder Diffraction File card.** No. 4-0457, Broch (1933).

**Additional published patterns.** Milligan, Watt, and Rachford (1949) Nautov (1962), Schwarz (1963), and Gambino and Guare (1963).

**NBS sample.** The sample of yttrium vanadate was furnished by P. Lublin, General Telephone and Electronics Lab., Bayside, N. Y.

Analysis by that company showed no impurities greater than 0.005 percent.

The color of the sample was yellow white and it was optically positive with indices of refraction $N_e \sim 2.05$ and $N_o \sim 1.98$. Because of the fine particle size and extremely high indices, these values are approximate.

$I/I_{corundum} = 3.6$.

**Structural data.** Broch (1933) determined that yttrium vanadate has the zircon structure, the space group $D_{4h}^{19}$-$I4_1/amd$ (No. 141), and $4(YVO_4)$ per unit cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Broch (1933) | 7.140 | 6.191 |
| Milligan, Watt, and Rachford (1949) | 7.10 | 6.27 |
| Nautov (1962) | 7.114 | 6.258 |
| Schwarz (1963) | 7.123 | 6.291 |
| NBS, sample at 25°C | 7.1192 | 6.2898 |

The density of yttrium vanadate, calculated from the NBS lattice constants is 4.247 g/cm³ at 25°C.

Internal standard W, a = 3.16504 Å

$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 4.711 | 8 | 101 | 18.82 |
| 3.559 | 100 | 200 | 25.00 |
| 2.831 | 1 | 211 | 31.58 |
| 2.668 | 46 | 112 | 33.56 |
| 2.518 | 12 | 220 | 35.63 |
| 2.357 | 6 | 202 | 38.15 |
| 2.220 | 12 | 301 | 40.60 |
| 2.012 | 5 | 103 | 45.03 |
| 1.884 | 6 | 321 | 48.26 |
| 1.830 | 46 | 312 | 49.78 |
| 1.780 | 13 | 400 | 51.28 |
| 1.751 | 1 | 213 | 52.19 |
| 1.666 | 1 | 411 | 55.09 |
| 1.5915 | 8 | 420 | 57.89 |
| 1.5722 | 4 | 004 | 58.67 |
| 1.5485 | 1 | 402 | 59.66 |
| 1.4805 | 11 | 332 | 62.70 |
| 1.4381 | 7 | 204 | 64.77 |
| 1.3884 | 3 | 501 | 67.39 |
| 1.3334 | 7 | 224 | 70.57 |
| 1.2894 | <1 | 314 | 73.37 |
| 1.2761 | 7 | 512 | 74.25 |
| 1.2586 | 2 | 440 | 75.47 |
| 1.1865 | 5 | 600 | 80.96 |
| 1.1783 | 3 | 503,404 | 81.64 |
| 1.1699 | 1 | 215 | 82.35 |
| 1.1507 | 1 | 611 | 84.04 |
| 1.1383 | 7 | 532 | 85.17 |
| 1.1255 | 4 | 620 | 86.37 |
| 1.1189 | 5 | 424 | 87.01 |
| 1.0609 | 1 | 325 | 93.11 |
| 1.0466 | 1 | 631 | 94.78 |
| 1.0262 | 2 | 116 | 97.29 |
| 1.0218 | 2 | 613 | 97.84 |
| 1.0164 | 1 | 415 | 98.54 |
| 0.9873 | 2 | 640 | 102.55 |
| .9826 | 2 | 444,543 | 103.24 |
| .9662 | 1 | 721 | 105.73 |
| .9643 | 1 | 534 | 106.03 |
| .9589 | 5 | 712 | 106.88 |
| .9503 | 2 | 316 | 108.30 |
| .9472 | 3 | 604,633 | 108.81 |
| .9427 | 1 | 505 | 109.59 |
| .9153 | 3 | 624,703 | 114.61 |
| .8960 | 4 | 732 | 118.56 |
| .8897 | 2 | 800 | 119.93 |
| .8890 | 2 | 336 | 120.09 |
| .8745 | 1 | 811 | 123.47 |
| .8648 | 2 | 217 | 125.91 |
| .8633 | 2 | 820 | 126.31 |
| .8383 | 6 | 516 | 133.51 |
| .8362 | 5 | 644,653 | 134.19 |

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**Powder Diffraction File cards.** None.

**Additional published patterns.** None.

**NBS sample.** The sample of zirconium hydride was obtained as grade "R" from Metal Hydrides Inc., Beverly, Mass.
The sample was dark gray and opaque.

$I/I_{corundum} = 8.8$.

**Structural data.** Rundle, Shull, and Wollan (1952) determined that zirconium dihydride has a body-centered tetragonal structure and $2(ZrH_2)$ per unit cell. The constants of Hägg have been converted to a body-centered cell.

*Lattice constants*

| | *a*(Å) | *c*(Å) |
|---|---|---|
| Hägg (1930) | 3.517 | 4.449 |
| Rundle, Shull, and Wollan (1952) | 3.520 | 4.449 |
| NBS, sample at 25°C | 3.5199 | 4.4500 |

The density of zirconium hydride calculated from the NBS lattice constants is 5.616 g/cm$^3$ at 25°C.

Internal standard W, a = 3.16504 Å
$CuK\alpha_1$ $\lambda$ = 1.5405 Å; temp. 25 °C

| *d* (Å) | *I* | *hkl* | 2θ(°) |
|---|---|---|---|
| 2.7608 | 100 | 101 | 32.40 |
| 2.4886 | 28 | 110 | 36.06 |
| 2.2248 | 11 | 002 | 40.51 |
| 1.7599 | 11 | 200 | 51.91 |
| 1.6587 | 17 | 112 | 55.34 |
| 1.4843 | 20 | 211 | 62.51 |
| 1.3804 | 8 | 202 | 67.83 |
| 1.3666 | 7 | 103 | 68.61 |
| 1.2443 | 2 | 220 | 76.51 |
| 1.1346 | 4 | 301 | 85.51 |
| 1.1128 | 4 | 310 | 87.60 |
| 1.0863 | 3 | 222 | 90.32 |
| 1.0797 | 6 | 213 | 91.02 |
| 1.0155 | 2 | 114 | 98.66 |
| 0.9955 | 5 | 312 | 101.38 |
| .9537 | 3 | 321 | 107.73 |
| .9403 | 2 | 204 | 110.00 |
| .9204 | 2 | 303 | 113.63 |
| .8801 | 1 | 400 | 122.14 |
| .8628 | 2 | 105 | 126.45 |
| .8386 | 3 | 411 | 133.42 |
| .8294 | 3 | 330,224 | 136.46 |
| .8184 | 2 | 402 | 140.48 |
| .8156 | 4 | 323 | 141.63 |
| .7869 | 6 | 420,314 | 156.41 |

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Rundle, R. E., Shull, C. G., and Wollan, E. O. (1952). The crystal structure of thorium and zirconium dihydrides by x-ray and neutron diffraction, Acta Cryst. 5, 22-26.

## Antimony Terbium, SbTb (cubic)

Additional published patterns. Olcese (1961).

Structural data. Brixner (1960) determined that antimony terbium is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(SbTb) per unit cell. The atoms occupy the special positions:

Sb: 0 0 0 ;F.C.
Tb: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

*Lattice constants*

| | a(Å) |
|---|---|
| Brixner (1960) | 6.178 |
| Olcese (1961) | 6.181 |
| Iandelli (1961) | 6.180 |

The lattice constant used in this calculated pattern is the average value a = 6.180 Å.
The calculated density is 7.898 g/cm³.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.57 | 3 | 111 | 24.93 |
| 3.09 | 100 | 200 | 28.87 |
| 2.18 | 69 | 220 | 41.28 |
| 1.863 | 1 | 311 | 48.81 |
| 1.784 | 23 | 222 | 51.16 |
| 1.545 | 10 | 400 | 59.81 |
| 1.418 | <1 | 331 | 65.81 |
| 1.382 | 26 | 420 | 67.75 |
| 1.261 | 19 | 422 | 75.26 |
| 1.189 | 40 | 511 | 80.73 |
| 1.092 | 6 | 440 | 89.67 |
| 1.045 | <1 | 531 | 95.01 |
| 1.030 | 12 | 600 | 96.80 |
| 0.977 | 9 | 620 | 104.0 |
| .942 | <1 | 533 | 109.6 |
| .932 | 8 | 622 | 115.3 |
| .892 | 3 | 444 | 119.4 |
| .865 | <1 | 711 | 125.8 |
| .857 | 8 | 640 | 128.0 |
| .826 | 16 | 642 | 137.7 |
| .805 | <1 | 731 | 146.4 |

## Barium Selenide, BaSe (cubic)

Additional published pattern. Slattery (1925).

Structural data. Haase (1927) determined that barium selenide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(BaSe) per unit cell. The atoms occupy the special positions:

Ba: 0 0 0 ;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

The lattice constant used in this calculated pattern is a = 6.600 Å as reported by Miller, Komarek, and Cadoff (1960).
The calculated density is 4.997 g/cm³.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.81 | 13 | 111 | 23.32 |
| 3.30 | 100 | 200 | 27.00 |
| 2.33 | 70 | 220 | 38.55 |
| 1.990 | 5 | 311 | 45.54 |
| 1.905 | 23 | 222 | 47.69 |
| 1.650 | 10 | 400 | 55.66 |
| 1.514 | 2 | 331 | 61.15 |
| 1.476 | 27 | 420 | 62.92 |
| 1.347 | 19 | 422 | 69.74 |
| 1.270 | 1 | 511 | 74.66 |
| 1.167 | 6 | 440 | 82.63 |
| 1.116 | 1 | 531 | 87.33 |
| 1.100 | 12 | 600 | 88.89 |
| 1.044 | 8 | 620 | 95.14 |
| 1.006 | <1 | 533 | 99.86 |
| 0.995 | 7 | 622 | 101.4 |
| .953 | 2 | 444 | 107.9 |
| .924 | <1 | 711 | 112.9 |
| .915 | 6 | 640 | 114.6 |
| .882 | 12 | 642 | 121.7 |
| .859 | 1 | 731 | 127.4 |
| .825 | 2 | 800 | 138.0 |
| .806 | <1 | 733 | 145.6 |
| .800 | 13 | 820 | 148.5 |

## Beryllium Cobalt, BeCo (cubic)

**Structural data.** Misch (1936) determined that beryllium cobalt is isostructural with cesium chloride with the space group $O_h^1$-Pm3m (No. 221) and 1(BeCo) per unit cell. The atoms occupy the special positions:

Be: 0 0 0
Co: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 2.611 Å as reported by Misch (1936). The calculated density is 6.338 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 2.61 | 100 | 100 | 34.3 |
| 1.846 | 89 | 110 | 49.3 |
| 1.507 | 19 | 111 | 61.5 |
| 1.306 | 12 | 200 | 72.3 |
| 1.168 | 21 | 210 | 82.6 |
| 1.066 | 23 | 211 | 92.5 |
| 0.923 | 8 | 220 | 113.1 |
| .870 | 12 | 300 | 124.5 |
| .826 | 15 | 310 | 137.8 |
| .787 | 11 | 311 | 156.2 |

## Beryllium Palladium, BePd (cubic)

**Structural data.** Misch (1936) determined that beryllium palladium is isostructural with cesium chloride with the space group $O_h^1$-Pm3m (No. 221) and 1(BePd) per unit cell. The atoms occupy the special positions:

Be: 0 0 0
Pd: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 2.819 Å as reported by Misch (1936). The calculated density is 8.554 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 2.82 | 100 | 100 | 31.7 |
| 1.993 | 82 | 110 | 45.5 |
| 1.628 | 21 | 111 | 56.5 |
| 1.410 | 11 | 200 | 66.2 |
| 1.261 | 23 | 210 | 75.3 |
| 1.151 | 21 | 211 | 84.0 |
| 0.997 | 7 | 220 | 101.22 |
| .940 | 13 | 300 | 110.11 |
| .891 | 13 | 310 | 119.55 |
| .850 | 10 | 311 | 129.98 |
| .814 | 4 | 222 | 142.35 |

## Cadmium Cerium, CdCe (cubic)

**Powder Diffraction File card.** No. 2-1455, Iandelli and Botti (1937).

**Structural data.** Iandelli and Botti (1937) determined that cadmium cerium is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1(CdCe) per unit cell. The atoms occupy the special positions:

Cd: 0 0 0
Ce: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.865 Å as reported by Iandelli and Botti (1937).

The calculated density is 7.262 g/cm³.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.86 | 1 | 100 | 23.0 |
| 2.73 | 100 | 110 | 32.7 |
| 2.23 | <1 | 111 | 40.4 |
| 1.932 | 16 | 200 | 47.0 |
| 1.728 | <1 | 210 | 52.9 |
| 1.578 | 31 | 211 | 58.4 |
| 1.366 | 9 | 220 | 68.6 |
| 1.288 | <1 | 300 | 73.4 |
| 1.222 | 12 | 310 | 78.1 |
| 1.165 | <1 | 311 | 82.8 |
| 1.116 | 3 | 222 | 87.3 |
| 1.072 | <1 | 320 | 91.9 |
| 1.033 | 14 | 321 | 96.4 |
| 0.966 | 2 | 400 | 105.7 |
| .937 | <1 | 410 | 110.5 |
| .911 | 9 | 411 | 115.4 |
| .864 | 6 | 420 | 126.1 |
| .843 | <1 | 421 | 131.9 |
| .824 | 6 | 332 | 138.4 |
| .789 | 6 | 422 | 155.0 |

## Cadmium Lanthanum, CdLa (cubic)

**Powder Diffraction File card.** No. 2-0855, Iandelli and Botti (1937).

**Structural data.** Iandelli and Botti (1937) determined that cadmium lanthanum is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1(CdLa) per unit cell. The atoms occupy the special positions:

Cd: 0 0 0
La: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in the calculated pattern is a = 3.905 Å as reported by Iandelli and Botti (1937).

The calculated density is 7.008 g/cm³.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.90 | 1 | 100 | 22.8 |
| 2.76 | 100 | 110 | 32.4 |
| 2.25 | <1 | 111 | 40.0 |
| 1.952 | 16 | 200 | 46.5 |
| 1.746 | <1 | 210 | 52.3 |
| 1.594 | 31 | 211 | 57.8 |
| 1.381 | 9 | 220 | 67.8 |
| 1.302 | <1 | 300 | 72.6 |
| 1.235 | 12 | 310 | 77.2 |
| 1.177 | <1 | 311 | 81.7 |
| 1.127 | 3 | 222 | 86.2 |
| 1.044 | 14 | 321 | 95.1 |
| 0.976 | 2 | 400 | 104.2 |
| .947 | <1 | 410 | 108.8 |
| .920 | 8 | 411 | 113.6 |
| .873 | 5 | 420 | 123.8 |
| .852 | <1 | 421 | 129.4 |
| .833 | 6 | 332 | 135.4 |
| .797 | 6 | 422 | 150.2 |

**Powder Diffraction File card.** No. 2-1457, Iandelli and Botti (1937).

**Structural data.** landelli and Botti (1937) determined that cadmium praseodymium is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1(CdPr) unit cell. The atoms occupy the special positions:

Cd: 0 0 0
Pr: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.830 Å as reported by landelli and Botti (1937).

The calculated density is 7.486 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I*(*Peak height*) | *hkl* | 2θ(°) |
|---|---|---|---|
| 3.83 | 2 | 100 | 23.20 |
| 2.71 | 100 | 110 | 33.05 |
| 2.21 | <1 | 111 | 40.77 |
| 1.915 | 16 | 200 | 47.43 |
| 1.713 | <1 | 210 | 53.45 |
| 1.564 | 31 | 211 | 59.03 |
| 1.354 | 9 | 220 | 69.34 |
| 1.277 | <1 | 300 | 74.22 |
| 1.211 | 12 | 310 | 78.98 |
| 1.155 | <1 | 311 | 83.67 |
| 1.106 | 3 | 222 | 88.32 |
| 1.062 | <1 | 320 | 92.96 |
| 1.024 | 14 | 321 | 97.61 |
| 0.958 | 2 | 400 | 107.1 |
| .929 | <1 | 410 | 112.0 |
| .903 | 9 | 411 | 117.1 |
| .856 | 6 | 420 | 128.2 |
| .836 | <1 | 421 | 134.3 |
| .817 | 6 | 332 | 141.2 |



**Additional published pattern.** Oftedal (1927).

**Structural data.** Oftedal (1927) determined that calcium selenide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(CaSe) per unit cell. The atoms occupy the special positions:

Ca: 0 0 0 ;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

*Lattice constants*

| | *a*(Å) |
|---|---|
| Oftedal (1927) | 5.924 |
| Senff and Klemm (1939) | 5.924 |

The lattice constant used in this calculated pattern is a = 5.924 Å.

The calculated density is 3.803 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I*(*Peak height*) | *hkl* | 2θ(°) |
|---|---|---|---|
| 3.42 | 18 | 111 | 26.03 |
| 2.96 | 100 | 200 | 30.15 |
| 2.09 | 65 | 220 | 43.15 |
| 1.786 | 8 | 311 | 51.09 |
| 1.710 | 20 | 222 | 53.54 |
| 1.481 | 9 | 400 | 62.68 |
| 1.359 | 3 | 331 | 69.05 |
| 1.325 | 23 | 420 | 71.11 |
| 1.209 | 16 | 422 | 79.13 |
| 1.140 | 2 | 511 | 85.00 |
| 1.047 | 5 | 440 | 94.70 |
| 1.001 | 2 | 531 | 100.6 |
| 0.987 | 11 | 600 | 102.6 |
| .937 | 8 | 620 | 110.6 |
| .903 | <1 | 533 | 117.0 |
| .893 | 8 | 622 | 119.2 |
| .855 | 2 | 444 | 128.5 |
| .830 | 2 | 711 | 136.4 |
| .822 | 8 | 640 | 139.3 |
| .792 | 17 | 642 | 153.3 |

## Cerium Magnesium, CeMg (cubic)

**Powder Diffraction File card.** No. 9-61, Rossi (1934).

**Additional published pattern.** Nowotny (1942).

**Structural data.** Nowotny (1942) determined that cerium magnesium is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1(CeMg) per unit cell. The atoms occupy the special positions:

Ce: 0 0 0
Mg: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

*Lattice constants*

| | *a*(Å) |
|---|---|
| Rossi (1934) | 3.892 |
| Nowotny (1942) | 3.906 |

The calculations are based on the average value, a = 3.899 Å.

The calculated density is 4.606 g/cm³.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I*(*Peak height*) | *hkl* | 2$\theta$(°) |
|---|---|---|---|
| 3.90 | 62 | 100 | 22.8 |
| 2.76 | 100 | 110 | 32.4 |
| 2.25 | 17 | 111 | 40.0 |
| 1.950 | 16 | 200 | 46.5 |
| 1.744 | 21 | 210 | 52.4 |
| 1.592 | 31 | 211 | 57.9 |
| 1.378 | 9 | 220 | 67.9 |
| 1.300 | 9 | 300 | 72.7 |
| 1.233 | 12 | 310 | 77.3 |
| 1.176 | 5 | 311 | 81.9 |
| 1.126 | 3 | 222 | 86.4 |
| 1.081 | 4 | 320 | 90.8 |
| 1.042 | 14 | 321 | 95.3 |
| 0.975 | 1 | 400 | 104.4 |
| .946 | 6 | 410 | 109.1 |
| .919 | 8 | 411 | 113.9 |
| .894 | 3 | 331 | 118.9 |
| .872 | 5 | 420 | 124.1 |
| .851 | 6 | 421 | 129.7 |
| .831 | 5 | 332 | 135.8 |
| .796 | 6 | 422 | 150.8 |

## Cerium Zinc, CeZn (cubic)

**Powder Diffraction File card.** No. 2-0974, Iandelli and Botti (1937).

**Structural data.** Iandelli and Botti (1937) determined that cerium zinc is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1(CeZn) per unit cell. The atoms occupy the special positions:

Ce: 0 0 0
Zn: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.704 Å as reported by Iandelli and Botti (1937).

The calculated density is 6.714 g/cm³.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I*(*Peak height*) | *hkl* | 2$\theta$(°) |
|---|---|---|---|
| 3.70 | 15 | 100 | 24.0 |
| 2.62 | 100 | 110 | 34.2 |
| 2.14 | 4 | 111 | 42.2 |
| 1.852 | 16 | 200 | 49.2 |
| 1.656 | 5 | 210 | 55.4 |
| 1.512 | 29 | 211 | 61.2 |
| 1.310 | 8 | 220 | 72.1 |
| 1.235 | 2 | 300 | 77.2 |
| 1.171 | 11 | 310 | 82.2 |
| 1.117 | 1 | 311 | 87.2 |
| 1.069 | 3 | 222 | 92.2 |
| 1.027 | 1 | 320 | 97.1 |
| 0.990 | 14 | 321 | 102.2 |
| .926 | 2 | 400 | 112.6 |
| .898 | 2 | 410 | 118.0 |
| .873 | 9 | 411 | 123.8 |
| .850 | <1 | 331 | 130.0 |
| .828 | 6 | 420 | 136.9 |
| .808 | 2 | 421 | 144.7 |
| .790 | 7 | 332 | 154.5 |

## Dysprosium Gold, DyAu (cubic)

**Structural data:** Chao, Luo, and Duwez (1963) reported that dysprosium gold is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1 (DyAu) per unit cell. The atoms occupy the special positions:

Dy: 0 0 0
Au: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.555 Å as reported by Chao, Luo, and Duwez (1963).

The calculated density is 13.28 g/cm$^3$.

Calculated Pattern
CuK$_{\alpha_1}$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I* (*Peak height*) | *hkl* | 2θ(°) |
|---|---|---|---|
| 3.56 | 1 | 100 | 25.03 |
| 2.51 | 100 | 110 | 35.69 |
| 2.05 | <1 | 111 | 44.08 |
| 1.778 | 16 | 200 | 51.36 |
| 1.590 | <1 | 210 | 57.96 |
| 1.451 | 30 | 211 | 64.11 |
| 1.257 | 9 | 220 | 75.59 |
| 1.185 | <1 | 300 | 81.08 |
| 1.124 | 12 | 310 | 86.50 |
| 1.072 | <1 | 311 | 91.88 |
| 1.026 | 3 | 222 | 97.28 |
| 0.986 | <1 | 320 | 102.7 |
| .950 | 17 | 321 | 108.3 |
| .889 | 2 | 400 | 120.2 |
| .862 | <1 | 410 | 126.6 |
| .838 | 8 | 411 | 133.6 |
| .816 | <1 | 331 | 141.6 |
| .795 | 9 | 420 | 151.4 |

## Dysprosium Silver, DyAg (cubic)

**Structural data.** Baenziger and Moriarty (1961) determined that dysprosium silver is isostructural with cesium chloride with the space group $O_h^1$-Pm3m (No. 221) and 1(DyAg) per unit cell. The atoms occupy the special positions:

Ag: 0 0 0
Dy: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.608 Å as reported by Baenziger and Moriarty (1961).

The calculated density is 9.558 g/cm$^3$.

Calculated Pattern
CuK$_{\alpha_1}$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I* (*Peak height*) | *hkl* | 2θ(°) |
|---|---|---|---|
| 3.61 | 4 | 100 | 24.65 |
| 2.55 | 100 | 110 | 35.14 |
| 2.08 | 1 | 111 | 43.40 |
| 1.804 | 15 | 200 | 50.55 |
| 1.614 | 2 | 210 | 57.03 |
| 1.473 | 29 | 211 | 63.06 |
| 1.276 | 8 | 220 | 74.29 |
| 1.203 | <1 | 300 | 79.65 |
| 1.141 | 11 | 310 | 84.92 |
| 1.088 | <1 | 311 | 90.15 |
| 1.042 | 3 | 222 | 95.38 |
| 1.001 | <1 | 320 | 100.66 |
| 0.964 | 15 | 321 | 106.03 |
| .902 | 2 | 400 | 117.28 |
| .875 | <1 | 410 | 123.34 |
| .850 | 10 | 411 | 129.8 |
| .828 | <1 | 331 | 137.0 |
| .807 | 7 | 420 | 145.4 |
| .787 | <1 | 421 | 156.1 |

## Erbium Silver, ErAg (cubic)

**Structural data:** Chao, Luo, and Duwez (1963) reported that erbium silver is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1(ErAg) per unit cell. The atoms occupy the special positions:

Er: 0 0 0
Ag: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

*Lattice constants*

| | *a*(Å) |
|---|---|
| Dwight (1959a) | 3.58 |
| Chao, et al. (1963) | 3.574 |

The lattice constant used in this calculated pattern is the average value a = 3.577 Å.

The calculated density is 9.98 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I*(*Peak height*) | *hkl* | 2$\theta$(°) |
|---|---|---|---|
| 3.57 | 5 | 100 | 24.9 |
| 2.53 | 100 | 110 | 35.5 |
| 2.06 | 1 | 111 | 43.8 |
| 1.787 | 15 | 200 | 51.1 |
| 1.598 | 2 | 210 | 57.6 |
| 1.459 | 28 | 211 | 63.7 |
| 1.264 | 8 | 220 | 75.1 |
| 1.191 | <1 | 300 | 80.6 |
| 1.130 | 11 | 310 | 85.9 |
| 1.078 | <1 | 311 | 91.2 |
| 1.032 | 3 | 222 | 96.6 |
| 0.991 | <1 | 320 | 102.0 |
| .955 | 15 | 321 | 107.5 |
| .894 | 2 | 400 | 119.1 |
| .867 | <1 | 410 | 125.4 |
| .842 | 11 | 411 | 132.2 |
| .820 | <1 | 331 | 139.9 |
| .799 | 8 | 420 | 149.1 |

## Gadolinium Indium, GdIn (cubic)

**Structural data:** Baenziger and Moriarty (1961) reported that gadolinium indium is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1(GdIn) per unit cell. The atoms occupy the special positions:

Gd: 0 0 0
In : $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.830 Å as reported by Baenziger and Moriarty (1961).

The calculated density is 8.041 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I*(*Peak height*) | *hkl* | 2$\theta$(°) |
|---|---|---|---|
| 3.83 | 3 | 100 | 23.20 |
| 2.71 | 100 | 110 | 33.05 |
| 2.21 | <1 | 111 | 40.77 |
| 1.915 | 16 | 200 | 47.43 |
| 1.713 | <1 | 210 | 53.45 |
| 1.564 | 31 | 211 | 59.03 |
| 1.354 | 9 | 220 | 69.34 |
| 1.277 | <1 | 300 | 74.22 |
| 1.211 | 12 | 310 | 78.98 |
| 1.155 | <1 | 311 | 83.67 |
| 1.106 | 3 | 222 | 88.32 |
| 1.062 | <1 | 320 | 92.96 |
| 1.024 | 15 | 321 | 97.61 |
| 0.958 | 2 | 400 | 107.1 |
| .929 | <1 | 410 | 112.0 |
| .903 | 9 | 411 | 117.1 |
| .879 | <1 | 331 | 122.5 |
| .856 | 6 | 420 | 128.2 |
| .836 | <1 | 421 | 134.3 |
| .817 | 6 | 332 | 141.2 |

## Gold Holmium, AuHo (cubic)

**Structural data.** Dwight (1961) reported that gold holmium is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1 (AuHo) per unit cell. The atoms occupy the special positions:

Au: 0 0 0
Ho: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

*Lattice constants*

| | a(Å) |
|---|---|
| Dwight (1961) | 3.549 |
| Chao, et al. (1963) | 3.541 |

The lattice constant used in this calculated pattern is the average value a = 3.545 Å.

The calculated density is 13.49 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.54 | 1 | 100 | 25.1 |
| 2.50 | 100 | 110 | 35.8 |
| 2.04 | <1 | 111 | 44.3 |
| 1.770 | 16 | 200 | 51.6 |
| 1.584 | <1 | 210 | 58.2 |
| 1.446 | 30 | 211 | 64.4 |
| 1.252 | 9 | 220 | 75.9 |
| 1.180 | <1 | 300 | 81.5 |
| 1.120 | 12 | 310 | 86.9 |
| 1.068 | <1 | 311 | 92.4 |
| 1.022 | 3 | 222 | 97.8 |
| 0.946 | 17 | 321 | 109.0 |
| .885 | 2 | 400 | 120.9 |
| .859 | <1 | 410 | 127.5 |
| .835 | 12 | 411 | 134.7 |
| .792 | 9 | 420 | 153.2 |

## Holmium Silver, HoAg (cubic)

**Structural data.** Walline and Wallace (1964) determined that holmium silver is isostructural with cesium chloride with the space group $O_h^1$-Pm3m (No. 221) and 1(HoAg) per unit cell. The atoms occupy the special positions:

Ag: 0 0 0
Ho: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is the average value a = 3.593 Å.

The calculated density is 9.765 g/cm$^3$.

*Lattice constants*

| | a(Å) |
|---|---|
| Dwight (1959a) | 3.594 |
| Chao, et al. (1963) | 3.592 |

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.59 | 4 | 100 | 24.76 |
| 2.54 | 100 | 110 | 35.31 |
| 2.07 | 1 | 111 | 43.61 |
| 1.79 | 15 | 200 | 50.79 |
| 1.606 | 2 | 210 | 57.30 |
| 1.466 | 29 | 211 | 63.37 |
| 1.270 | 8 | 220 | 74.68 |
| 1.197 | <1 | 300 | 80.08 |
| 1.136 | 11 | 310 | 85.39 |
| 1.083 | <1 | 311 | 90.67 |
| 1.037 | 3 | 222 | 95.95 |
| 0.996 | <1 | 320 | 101.3 |
| .960 | 15 | 321 | 106.7 |
| .898 | 2 | 400 | 118.1 |
| .871 | <1 | 410 | 124.3 |
| .847 | 11 | 411 | 131.0 |
| .824 | <1 | 331 | 138.4 |
| .803 | 8 | 420 | 147.1 |
| .784 | <1 | 421 | 158.6 |

**Powder Diffraction File card.** No. 9-241, Rossi (1934).

**Additional published pattern.** Nowotny (1942).

**Structural data.** Nowotny (1942) determined that lanthanum magnesium is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1(LaMg) per unit cell. The atoms occupy the special positions:

La: 0 0 0
Mg: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

*Lattice constants*

| | a(Å) |
|---|---|
| Rossi (1934) | 3.960 |
| Nowotny (1942) | 3.973 |

The calculations are based on the average value, a = 3.966 Å.

The calculated density is 4.345 g/cm³.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.97 | 62 | 100 | 22.40 |
| 2.80 | 100 | 110 | 31.88 |
| 2.29 | 16 | 111 | 39.31 |
| 1.983 | 16 | 200 | 45.71 |
| 1.774 | 20 | 210 | 51.48 |
| 1.619 | 31 | 211 | 56.81 |
| 1.402 | 9 | 220 | 66.64 |
| 1.322 | 9 | 300 | 71.27 |
| 1.254 | 12 | 310 | 75.78 |
| 1.196 | 5 | 311 | 80.20 |
| 1.145 | 3 | 222 | 84.56 |
| 1.100 | 4 | 320 | 88.89 |
| 1.060 | 14 | 321 | 93.22 |
| 0.992 | 1 | 400 | 102.0 |
| .962 | 6 | 410 | 106.4 |
| .935 | 8 | 411 | 111.0 |
| .910 | 3 | 331 | 115.7 |
| .887 | 5 | 420 | 120.6 |
| .865 | 5 | 421 | 125.8 |
| .846 | 5 | 332 | 131.3 |
| .810 | 5 | 422 | 144.2 |
| .793 | 4 | 500 | 152.4 |



**Additional published pattern.** Iandelli and Botti (1936).

**Structural data.** Iandelli and Botti (1936) determined that lanthanum phosphide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(LaP) per unit cell. The atoms occupy the special positions:

La: 0 0 0 ;F.C.
P: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

The lattice constant used in this calculated pattern is a = 6.025 Å as reported by Iandelli and Botti (1936).

The calculated density is 5.159 g/cm³.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.48 | 78 | 111 | 25.6 |
| 3.01 | 100 | 200 | 29.6 |
| 2.13 | 66 | 220 | 42.4 |
| 1.817 | 32 | 311 | 50.2 |
| 1.739 | 22 | 222 | 52.6 |
| 1.506 | 10 | 400 | 61.5 |
| 1.382 | 12 | 331 | 67.7 |
| 1.347 | 25 | 420 | 69.7 |
| 1.230 | 18 | 422 | 77.6 |
| 1.160 | 8 | 511 | 83.3 |
| 1.065 | 6 | 440 | 92.6 |
| 1.018 | 9 | 531 | 98.3 |
| 1.004 | 12 | 600 | 100.2 |
| 0.953 | 9 | 620 | 107.9 |
| .919 | 4 | 533 | 113.9 |
| .908 | 9 | 622 | 116.0 |
| .870 | 3 | 444 | 124.7 |
| .844 | 7 | 711 | 131.8 |
| .836 | 8 | 640 | 134.4 |
| .805 | 17 | 642 | 146.2 |
| .784 | 13 | 731 | 158.2 |

**Powder Diffraction File card.** No. 2-1460, Iandelli and Botti (1937).

**Structural data.** Iandelli and Botti (1937) determined that lanthanum zinc is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1(LaZn) per unit cell. The atoms occupy the special positions:

La: 0 0 0
Zn: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.760 Å as reported by Iandelli and Botti (1937).

The calculated density is 6.381 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.76 | 14 | 100 | 23.64 |
| 2.66 | 100 | 110 | 33.68 |
| 2.17 | 4 | 111 | 41.56 |
| 1.880 | 16 | 200 | 48.37 |
| 1.682 | 5 | 210 | 54.52 |
| 1.535 | 30 | 211 | 60.24 |
| 1.329 | 9 | 220 | 70.82 |
| 1.253 | 2 | 300 | 75.84 |
| 1.189 | 11 | 310 | 80.75 |
| 1.134 | 1 | 311 | 85.60 |
| 1.085 | 3 | 222 | 90.41 |
| 1.043 | 1 | 320 | 95.23 |
| 1.005 | 14 | 321 | 100.1 |
| 0.940 | 2 | 400 | 110.0 |
| .912 | 2 | 410 | 115.3 |
| .886 | 9 | 411 | 120.7 |
| .863 | <1 | 331 | 126.5 |
| .841 | 6 | 420 | 132.7 |
| .820 | 2 | 421 | 139.7 |
| .802 | 6 | 332 | 147.8 |



**Additional published pattern.** Broch (1927).

**Structural data.** Broch (1927) determined that magnesium selenide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(MgSe) per unit cell. The atoms occupy the special positions:

Mg: 0 0 0 ;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

The lattice constant used in this calculated pattern is a = 5.462 Å as reported by Broch (1927).

The calculated density is 4.209 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.15 | 54 | 111 | 28.3 |
| 2.73 | 100 | 200 | 32.8 |
| 1.931 | 64 | 220 | 47.0 |
| 1.647 | 19 | 311 | 55.8 |
| 1.577 | 20 | 222 | 58.5 |
| 1.366 | 9 | 400 | 68.7 |
| 1.253 | 7 | 331 | 75.9 |
| 1.221 | 22 | 420 | 78.2 |
| 1.115 | 16 | 422 | 87.4 |
| 1.051 | 6 | 511 | 94.2 |
| 0.966 | 5 | 440 | 105.8 |
| .923 | 7 | 531 | 113.1 |
| .910 | 13 | 600 | 115.6 |
| .864 | 10 | 620 | 126.2 |
| .833 | 3 | 533 | 135.2 |
| .823 | 9 | 622 | 138.6 |
| .788 | 4 | 444 | 155.4 |

## Neodymium Selenide, NdSe (cubic)

**Structural data.** Iandelli (1955) determined that neodymium selenide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(NdSe) per unit cell. The atoms occupy the special positions:

Nd: 0 0 0 ;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

*Lattice constants*

| | a(Å) |
|---|---|
| Iandelli (1955) | 5.909 |
| Guittard and Benecerraf (1959) | 5.891 |

The lattice constant used in this calculated pattern is the average value a = 5.900 Å.

The calculated density is 7.218 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.41 | 16 | 111 | 26.1 |
| 2.95 | 100 | 200 | 30.3 |
| 2.09 | 67 | 220 | 43.3 |
| 1.779 | 7 | 311 | 51.3 |
| 1.703 | 22 | 222 | 53.8 |
| 1.475 | 9 | 400 | 63.0 |
| 1.354 | 2 | 331 | 69.4 |
| 1.319 | 25 | 420 | 71.4 |
| 1.204 | 18 | 422 | 79.5 |
| 1.135 | 2 | 511 | 85.4 |
| 1.043 | 6 | 440 | 95.2 |
| 0.997 | 2 | 531 | 101.1 |
| .983 | 13 | 600 | 103.1 |
| .933 | 9 | 620 | 111.3 |
| .900 | <1 | 533 | 117.8 |
| .889 | 9 | 622 | 120.0 |
| .852 | 3 | 444 | 129.5 |
| .826 | 2 | 711 | 137.6 |
| .818 | 9 | 640 | 140.6 |
| .788 | 20 | 642 | 155.4 |

## Neodymium Silver, NdAg (cubic)

**Structural data.** Iandelli (1960) reported that neodymium silver is isostructural with cesium chloride with the space group $O_h^1$-Pm3m (No. 221) and 1(NdAg) per unit cell. The atoms occupy the special positions:

Nd: 0 0 0
Ag: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

*Lattice constants*

| | a(Å) |
|---|---|
| Dwight (1959a) | 3.722 |
| Iandelli (1960) | 3.711 |
| Ferro (1955) | 3.714 |

The lattice constant used in this calculated pattern is the average value a = 3.716 Å.

The calculated density is 8.158 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.71 | 2 | 100 | 23.9 |
| 2.63 | 100 | 110 | 34.1 |
| 2.14 | <1 | 111 | 42.1 |
| 1.857 | 16 | 200 | 49.0 |
| 1.661 | <1 | 210 | 55.3 |
| 1.516 | 29 | 211 | 61.1 |
| 1.313 | 8 | 220 | 71.8 |
| 1.238 | <1 | 300 | 77.0 |
| 1.174 | 11 | 310 | 82.0 |
| 1.120 | <1 | 311 | 86.9 |
| 1.072 | 3 | 222 | 91.9 |
| 1.030 | <1 | 320 | 96.8 |
| 0.993 | 14 | 321 | 101.8 |
| .928 | 2 | 400 | 112.1 |
| .901 | <1 | 410 | 117.5 |
| .875 | 9 | 411 | 123.3 |
| .852 | <1 | 331 | 129.4 |
| .830 | 6 | 420 | 136.1 |
| .810 | <1 | 421 | 143.8 |
| .792 | 7 | 332 | 153.2 |

## Palladium Hydride, $PdH_{0.706}$ (cubic)

**Structural data.** Worsham, Wilkinson, and Shull (1957) determined that palladium hydride is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(PdH) per unit cell. The atoms occupy the special positions:

Pd: 0 0 0 ;F.C.
H: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$ ;F.C.

The lattice constant used in this calculated pattern is a = 4.02 Å as reported by Worsham, Wilkinson, and Shull (1957).

The calculated density is 11.0 g/cm³.

Calculated Pattern
$CuK_{\alpha_1}$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I*(*Peak height*) | *hkl* | 2θ(°) |
|---|---|---|---|
| 2.32 | 100 | 111 | 38.8 |
| 2.01 | 49 | 200 | 45.1 |
| 1.42 | 26 | 220 | 65.6 |
| 1.21 | 29 | 311 | 78.9 |
| 1.16 | 8 | 222 | 83.2 |
| 1.00 | 4 | 400 | 100.1 |
| 0.922 | 15 | 331 | 113.3 |
| .899 | 14 | 420 | 117.9 |
| .821 | 14 | 422 | 139.7 |

## Praseodymium Zinc, PrZn (cubic)

**Powder Diffraction File card.** No. 2-0994, Iandelli and Botti (1937).

**Structural data.** Iandelli and Botti (1937) determined that praseodymium zinc is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1(PrZn) per unit cell. The atoms occupy the special positions:

Pr: 0 0 0
Zn: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.678 Å as reported by Iandelli and Botti (1937).

The calculated density is 6.884 g/cm³.

Calculated Pattern
$CuK_{\alpha_1}$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I*(*Peak height*) | *hkl* | 2θ(°) |
|---|---|---|---|
| 3.68 | 16 | 100 | 24.2 |
| 2.60 | 100 | 110 | 34.4 |
| 2.12 | 4 | 111 | 42.5 |
| 1.839 | 16 | 200 | 49.5 |
| 1.645 | 5 | 210 | 55.8 |
| 1.501 | 29 | 211 | 61.7 |
| 1.300 | 8 | 220 | 72.6 |
| 1.226 | 2 | 300 | 77.8 |
| 1.163 | 11 | 310 | 82.9 |
| 1.109 | 1 | 311 | 88.0 |
| 1.062 | 3 | 222 | 93.0 |
| 1.020 | 1 | 320 | 98.1 |
| 0.983 | 15 | 321 | 103.2 |
| .920 | 2 | 400 | 113.8 |
| .892 | 2 | 410 | 119.4 |
| .867 | 9 | 411 | 125.4 |
| .844 | 1 | 331 | 131.8 |
| .822 | 7 | 420 | 139.0 |
| .803 | 2 | 421 | 147.4 |
| .784 | 8 | 332 | 158.4 |

## Rubidium Amide, $RbNH_2$ at 50°C (cubic)

**Powder Diffraction File card.** No. 12-748, Juza and Mehne (1959).

**Structural data.** Juza and Mehne (1959) determined that rubidium amide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4($RbNH_2$) per unit cell. The atoms occupy the special positions:

Rb: 0 0 0 ;F.C.
N: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.
H: Undetermined

The lattice constant used in this calculated pattern is a = 6.395 Å as reported by Juza and Mehne (1959).
The calculated density is 2.577 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I*(*Peak height*) | *hkl* | 2θ(°) |
|---|---|---|---|
| 3.69 | 100 | 111 | 24.08 |
| 3.20 | 100 | 200 | 27.88 |
| 2.26 | 65 | 220 | 39.84 |
| 1.928 | 42 | 311 | 47.09 |
| 1.846 | 21 | 222 | 49.32 |
| 1.599 | 9 | 400 | 57.60 |
| 1.467 | 15 | 331 | 63.34 |
| 1.430 | 23 | 420 | 65.18 |
| 1.305 | 16 | 422 | 72.32 |
| 1.231 | 11 | 511 | 77.49 |
| 1.130 | 5 | 440 | 85.90 |
| 1.081 | 11 | 531 | 90.89 |
| 1.066 | 10 | 600 | 92.55 |
| 1.011 | 7 | 620 | 99.24 |
| 0.975 | 4 | 533 | 104.3 |
| .964 | 6 | 622 | 106.1 |
| .923 | 2 | 444 | 113.1 |
| .895 | 7 | 711 | 118.7 |
| .887 | 6 | 640 | 120.6 |
| .855 | 11 | 642 | 128.7 |
| .833 | 11 | 731 | 135.4 |
| .799 | 2 | 800 | 149.0 |

## Samarium Silver, SmAg (cubic)

**Structural data:** Walline and Wallace (1964) reported that samarium silver is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1(SmAg) per unit cell. The atoms occupy the special positions:

Sm: 0 0 0
Ag: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

*Lattice constants*

| | *a*(Å) |
|---|---|
| Dwight (1959a) | 3.678 |
| Iandelli (1960) | 3.684 |
| Chao, et al. (1963) | 3.673 |

The lattice constant used in this calculated pattern is the average value a = 3.678 Å.
The calculated density is 8.617 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I*(*Peak height*) | *hkl* | 2θ(°) |
|---|---|---|---|
| 3.67 | 3 | 100 | 24.2 |
| 2.60 | 100 | 110 | 34.5 |
| 2.12 | <1 | 111 | 42.6 |
| 1.836 | 16 | 200 | 49.6 |
| 1.643 | 1 | 210 | 55.9 |
| 1.500 | 29 | 211 | 61.8 |
| 1.299 | 8 | 220 | 72.8 |
| 1.224 | <1 | 300 | 78.0 |
| 1.162 | 11 | 310 | 83.1 |
| 1.107 | <1 | 311 | 88.1 |
| 1.060 | 3 | 222 | 93.2 |
| 1.019 | <1 | 320 | 98.2 |
| 0.982 | 15 | 321 | 103.4 |
| .918 | 2 | 400 | 114.0 |
| .891 | <1 | 410 | 119.7 |
| .866 | 10 | 411 | 125.7 |
| .843 | <1 | 331 | 132.2 |
| .821 | 7 | 420 | 139.4 |
| .802 | <1 | 421 | 147.9 |
| .783 | 8 | 332 | 159.2 |

## Silver Terbium, AgTb (cubic)

Structural data: Walline and Wallace (1964) reported that silver terbium is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m (No. 221) and 1(AgTb) per unit cell. The atoms occupy the special positions:

Ag: 0 0 0
Tb: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.625 Å as reported by Chao, Luo, and Duwez (1963).

The calculated density is 9.300 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.62 | 4 | 100 | 24.54 |
| 2.56 | 100 | 110 | 34.97 |
| 2.09 | 1 | 111 | 43.19 |
| 1.812 | 15 | 200 | 50.30 |
| 1.621 | 1 | 210 | 56.74 |
| 1.480 | 29 | 211 | 62.73 |
| 1.282 | 8 | 220 | 73.88 |
| 1.208 | <1 | 300 | 79.20 |
| 1.146 | 11 | 310 | 84.43 |
| 1.093 | <1 | 311 | 89.61 |
| 1.046 | 3 | 222 | 94.79 |
| 1.005 | <1 | 320 | 100.0 |
| 0.969 | 15 | 321 | 105.3 |
| .906 | 2 | 400 | 116.4 |
| .879 | <1 | 410 | 122.4 |
| .854 | 10 | 411 | 128.7 |
| .832 | <1 | 331 | 135.7 |
| .811 | 7 | 420 | 143.7 |
| .791 | <1 | 421 | 153.7 |

## Silver Thulium, AgTm (cubic)

Structural data: Chao, Luo, and Duwez (1963) reported that silver thulium is isostructural with cesium chloride, with the space group $O_h^1$-Pm3m(No. 221) and 1(AgTm) per unit cell. The atoms occupy the special positions:

Ag: 0 0 0
Tm: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$

The lattice constant used in this calculated pattern is a = 3.562 Å as reported by Chao, Luo, and Duwez (1963).

The calculated density is 10.17 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.56 | 5 | 100 | 24.98 |
| 2.52 | 100 | 110 | 35.61 |
| 2.06 | 2 | 111 | 43.99 |
| 1.781 | 16 | 200 | 51.25 |
| 1.593 | 2 | 210 | 57.83 |
| 1.454 | 29 | 211 | 63.97 |
| 1.259 | 8 | 220 | 75.41 |
| 1.187 | 1 | 300 | 80.89 |
| 1.126 | 11 | 310 | 86.28 |
| 1.074 | <1 | 311 | 91.65 |
| 1.028 | 3 | 222 | 97.02 |
| 0.988 | <1 | 320 | 102.5 |
| .952 | 5 | 321 | 108.0 |
| .890 | 2 | 400 | 119.8 |
| .864 | <1 | 410 | 126.2 |
| .840 | 7 | 411 | 133.1 |
| .817 | <1 | 331 | 141.0 |
| .796 | 8 | 420 | 150.5 |

## Silver Yttrium, AgY (cubic)

**Structural data.** Moriarty et al. (1966) reported that silver yttrium is isostructural with cesium chloride with the space group $O_h^1$-Pm3m (No. 221) and 1(AgY) per unit cell. The atoms occupy the special positions:

Ag: 0 0 0
Y: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

*Lattice constants*

| | a(Å) |
|---|---|
| Dwight (1959b) | 3.617 |
| Bruzzone, et al. (1962) | 3.619 |
| Moriarty, et al. (1966) | 3.6196 |

The lattice constant used in this calculated pattern is a = 3.6196 Å as reported by Moriarty et al. (1966).

The calculated density is 6.890 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.62 | 1 | 100 | 24.6 |
| 2.56 | 100 | 110 | 35.0 |
| 2.09 | <1 | 111 | 43.3 |
| 1.808 | 15 | 200 | 50.4 |
| 1.618 | <1 | 210 | 56.8 |
| 1.477 | 27 | 211 | 62.8 |
| 1.279 | 8 | 220 | 74.1 |
| 1.206 | 1 | 300 | 79.4 |
| 1.144 | 11 | 310 | 84.6 |
| 1.044 | 3 | 222 | 95.0 |
| 0.967 | 14 | 321 | 105.5 |
| .904 | 2 | 400 | 116.7 |
| .877 | 1 | 410 | 122.7 |
| .853 | 9 | 411 | 129.1 |
| .809 | 7 | 420 | 144.2 |
| .789 | <1 | 421 | 154.4 |

## Terbium Arsenide, TbAs (cubic)

**Additional published pattern.** Olcese (1961).

**Structural data.** Brixner (1960) determined that terbium arsenide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(TbAs) per unit cell. The atoms occupy the special positions:

Tb: 0 0 0 ;F.C.
As: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

*Lattice constants*

| | a(Å) |
|---|---|
| Brixner (1960) | 5.813 |
| Olcese (1961) | 5.827 |
| Iandelli (1961) | 5.827 |

The lattice constant used in this calculated pattern is the average value a = 5.822 Å.

The calculated density is 7.870 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.36 | 24 | 111 | 26.5 |
| 2.91 | 100 | 200 | 30.7 |
| 2.06 | 88 | 220 | 44.0 |
| 1.755 | 13 | 311 | 52.1 |
| 1.680 | 29 | 222 | 54.6 |
| 1.455 | 13 | 400 | 63.9 |
| 1.335 | 5 | 331 | 70.5 |
| 1.301 | 33 | 420 | 72.6 |
| 1.188 | 24 | 422 | 80.8 |
| 1.120 | 4 | 511 | 86.9 |
| 1.029 | 8 | 440 | 97.0 |
| 0.984 | 4 | 531 | 103.1 |
| .970 | 17 | 600 | 105.1 |
| .920 | 13 | 620 | 113.6 |
| .888 | 2 | 533 | 120.4 |
| .877 | 13 | 622 | 122.8 |
| .840 | 4 | 444 | 133.0 |
| .815 | 4 | 711 | 141.9 |
| .807 | 13 | 640 | 145.2 |

## Terbium Phosphide, TbP (cubic)

Additional published pattern. Olcese (1961).

Structural data. Olcese (1961) determined that terbium phosphide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(TbP) per unit cell. The atoms occupy the special positions:

Tb: 0 0 0;F.C.
P: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

*Lattice constants*

| | a(Å) |
|---|---|
| Iandelli (1961) | 5.686 |
| Olcese (1961) | 5.688 |

The lattice constant used in this calculated pattern is the average value a = 5.687 Å.

The calculated density is 6.857 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.28 | 89 | 111 | 27.1 |
| 2.84 | 100 | 200 | 31.4 |
| 2.01 | 66 | 220 | 45.0 |
| 1.715 | 35 | 311 | 53.4 |
| 1.642 | 21 | 222 | 56.0 |
| 1.422 | 9 | 400 | 65.6 |
| 1.305 | 13 | 331 | 72.4 |
| 1.272 | 24 | 420 | 74.6 |
| 1.161 | 18 | 422 | 83.1 |
| 1.095 | 9 | 511 | 89.5 |
| 1.006 | 6 | 440 | 100.0 |
| 0.961 | 11 | 531 | 106.5 |
| .948 | 14 | 600 | 108.7 |
| .899 | 10 | 620 | 117.9 |
| .867 | 5 | 533 | 125.3 |
| .858 | 10 | 622 | 127.9 |
| .821 | 3 | 444 | 139.6 |
| .796 | 11 | 711 | 150.6 |
| .789 | 12 | 640 | 155.2 |

## Terbium Selenide, TbSe (cubic)

Additional published pattern. Olcese (1961).

Structural data. Olcese (1961) determined that terbium selenide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(TbSe) per unit cell. The atoms occupy the special positions:

Tb: 0 0 0;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$;F.C.

*Lattice constants*

| | a(Å) |
|---|---|
| Iandelli (1961) | 5.740 |
| Olcese (1961) | 5.741 |

The lattice constant used in this calculated pattern is a = 5.741 Å.

The calculated density is 8.350 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.31 | 22 | 111 | 26.87 |
| 2.87 | 100 | 200 | 31.13 |
| 2.03 | 66 | 220 | 44.60 |
| 1.731 | 9 | 311 | 52.84 |
| 1.657 | 22 | 222 | 55.39 |
| 1.435 | 9 | 400 | 64.91 |
| 1.317 | 3 | 331 | 71.58 |
| 1.284 | 25 | 420 | 73.74 |
| 1.172 | 18 | 422 | 82.19 |
| 1.105 | 2 | 511 | 88.40 |
| 1.015 | 6 | 440 | 98.75 |
| 0.970 | 3 | 531 | 105.1 |
| .957 | 14 | 600 | 107.2 |
| .908 | 10 | 620 | 116.1 |
| .875 | 1 | 533 | 123.2 |
| .865 | 10 | 622 | 125.7 |
| .829 | 3 | 444 | 136.7 |
| .804 | 3 | 711 | 146.7 |
| .796 | 10 | 640 | 150.7 |

## Terbium Sulfide, TbS (cubic)

Additional published pattern. Olcese (1961).

**Structural data.** Olcese (1961) determined that terbium sulfide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(TbS) per unit cell. The atoms occupy the special positions:

Tb: 0 0 0 ;F.C.
S: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

*Lattice constants*

| | a(Å) |
|---|---|
| Iandelli (1961) | 5.517 |
| Olcese (1961) | 5.516 |

The lattice constant used in this calculated pattern is a = 5.516 Å.

The calculated density is 7.558 g/cm³.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.18 | 83 | 111 | 27.99 |
| 2.76 | 100 | 200 | 32.43 |
| 1.950 | 63 | 220 | 46.53 |
| 1.663 | 33 | 311 | 55.18 |
| 1.592 | 20 | 222 | 57.86 |
| 1.379 | 9 | 400 | 67.91 |
| 1.265 | 12 | 331 | 74.99 |
| 1.233 | 23 | 420 | 77.29 |
| 1.126 | 18 | 422 | 86.33 |
| 1.062 | 9 | 511 | 93.04 |
| 0.975 | 6 | 440 | 104.4 |
| .932 | 11 | 531 | 111.4 |
| .919 | 14 | 600 | 113.8 |
| .872 | 11 | 620 | 124.0 |
| .841 | 5 | 533 | 132.6 |
| .832 | 11 | 622 | 135.7 |
| .796 | 4 | 444 | 150.7 |

## Terbium Telluride, TbTe (cubic)

Additional published pattern. Olcese (1961).

**Structural data.** Brixner (1960) determined that terbium telluride is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(TbTe) per unit cell. The atoms occupy the special positions:

Tb: 0 0 0 ;F.C.
Te: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

*Lattice constants*

| | a(Å) |
|---|---|
| Brixner (1960) | 6.101 |
| Iandelli (1961) | 6.101 |
| Olcese (1961) | 6.102 |

The lattice constant used in this calculated pattern is a = 6.101 Å.

The calculated density is 8.380 g/cm³.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.52 | 3 | 111 | 25.26 |
| 3.05 | 100 | 200 | 29.25 |
| 2.16 | 68 | 220 | 41.84 |
| 1.840 | 1 | 311 | 49.50 |
| 1.762 | 22 | 222 | 51.86 |
| 1.526 | 10 | 400 | 60.65 |
| 1.400 | <1 | 331 | 66.76 |
| 1.364 | 26 | 420 | 68.74 |
| 1.246 | 19 | 422 | 76.40 |
| 1.174 | <1 | 511 | 81.98 |
| 1.079 | 6 | 440 | 91.13 |
| 1.031 | <1 | 531 | 96.62 |
| 1.017 | 13 | 600 | 98.47 |
| 0.965 | 9 | 620 | 105.9 |
| .931 | <1 | 533 | 111.7 |
| .920 | 8 | 622 | 113.7 |
| .881 | 3 | 444 | 122.0 |
| .854 | <1 | 711 | 128.7 |
| .846 | 8 | 640 | 131.1 |
| .815 | 17 | 642 | 141.7 |
| .794 | <1 | 731 | 151.7 |

## Uranium Oxide, UO (cubic)

**Structural data.** Rundle, Wilson, Baenziger, and Trevebaugh (1958) determined that uranium oxide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(UO) per unit cell. The atoms occupy the special positions:

U: 0 0 0 ;F.C.
O: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

The lattice constant used in this calculated pattern is a = 4.91 Å as reported by Rundle, Wilson, Baenziger, and Trevebaugh (1958).

The calculated density is 14.3 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I*(*Peak height*) | *hkl* | 2θ(°) |
|---|---|---|---|
| 2.83 | 100 | 111 | 31.5 |
| 2.46 | 66 | 200 | 36.6 |
| 1.74 | 41 | 220 | 52.7 |
| 1.48 | 36 | 311 | 62.7 |
| 1.42 | 13 | 222 | 65.8 |
| 1.23 | 6 | 400 | 77.7 |
| 1.13 | 15 | 331 | 86.3 |
| 1.10 | 16 | 420 | 89.1 |
| 1.00 | 13 | 422 | 100.4 |
| 0.945 | 13 | 511 | 109.2 |
| .868 | 5 | 440 | 125.1 |
| .830 | 19 | 531 | 136.3 |
| .818 | 15 | 600 | 140.5 |

## Uranium Selenide, USe (cubic)

**Structural data.** Ferro (1954) determined that uranium selenide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(USe) per unit cell. The atoms occupy the special positions:

U: 0 0 0 ;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

The lattice constant used in this calculated pattern is a = 5.751 Å as reported by Ferro (1954). Khodadad (1961) gives a = 5.66 Å.

The calculated density is 11.07 g/cm$^3$, based on the value a = 5.751 Å.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| *d*(Å) | *I*(*Peak height*) | *hkl* | 2θ(°) |
|---|---|---|---|
| 3.32 | 46 | 111 | 26.8 |
| 2.88 | 100 | 200 | 31.1 |
| 2.03 | 68 | 220 | 44.5 |
| 1.734 | 19 | 311 | 52.8 |
| 1.660 | 22 | 222 | 55.3 |
| 1.438 | 10 | 400 | 64.8 |
| 1.319 | 7 | 331 | 71.4 |
| 1.286 | 26 | 420 | 73.6 |
| 1.174 | 19 | 422 | 82.0 |
| 1.107 | 5 | 511 | 88.2 |
| 1.017 | 6 | 440 | 98.5 |
| 0.972 | 6 | 531 | 104.8 |
| .958 | 14 | 600 | 107.0 |
| .909 | 11 | 620 | 115.8 |
| .877 | 3 | 533 | 122.9 |
| .867 | 10 | 622 | 125.4 |
| .830 | 4 | 444 | 136.2 |
| .805 | 6 | 711 | 146.1 |
| .798 | 12 | 640 | 150.0 |

## Ytterbium Selenide, YbSe (cubic)

**Additional published pattern.** Senff and Klemm (1939).

**Structural data.** Senff and Klemm (1939) determined that ytterbium selenide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m and 4(YbSe) per unit cell. The atoms occupy the special positions:

Yb: 0 0 0 ;F.C.
Se: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

*Lattice constants*

| | a(Å) |
|---|---|
| Senff and Klemm (1939) | 5.879 |
| Iandelli (1961) | 5.931 |
| Miller, et al. (1962) | 5.94 |

Senff and Klemm (1939) identified the presence of 0.9 weight percent of an impurity. The lattice constant a = 5.935 Å used to calculate this pattern is an average of the last two values above.

The calculated density is 8.006 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.43 | 26 | 111 | 26.0 |
| 2.97 | 100 | 200 | 30.1 |
| 2.10 | 68 | 220 | 43.1 |
| 1.789 | 11 | 311 | 51.0 |
| 1.713 | 22 | 222 | 53.4 |
| 1.484 | 10 | 400 | 62.6 |
| 1.362 | 4 | 331 | 68.9 |
| 1.327 | 25 | 420 | 71.0 |
| 1.211 | 18 | 422 | 79.0 |
| 1.142 | 3 | 511 | 84.8 |
| 1.049 | 6 | 440 | 94.5 |
| 1.003 | 3 | 531 | 100.3 |
| 0.989 | 13 | 600 | 102.3 |
| .938 | 10 | 620 | 110.3 |
| .905 | 1 | 533 | 116.7 |
| .895 | 9 | 622 | 118.8 |
| .857 | 3 | 444 | 128.1 |
| .831 | 3 | 711 | 135.9 |
| .823 | 9 | 640 | 138.7 |
| .793 | 20 | 642 | 152.4 |

## Ytterbium Telluride, YbTe (cubic)

**Additional published pattern.** Senff and Klemm (1939).

**Structural data.** Senff and Klemm (1939) determined that ytterbium telluride is isostructural with sodium chloride, with the space group $O_h^5$-Fm3m (No. 225) and 4(YbTe) per unit cell. The atoms occupy the special positions:

Yb: 0 0 0 ;F.C.
Te: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

*Lattice constants*

| | a(Å) |
|---|---|
| Senff and Klemm (1939) | 6.353 |
| Iandelli (1961) | 6.361 |
| Miller, et al. (1962) | 6.37 |

Senff and Klemm (1939) identified the presence of 0.6 weight percent of an impurity. The lattice constant a = 6.365 Å used to calculate this pattern is an average of the last two values above.

The calculated density is 7.743 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.67 | 5 | 111 | 24.2 |
| 3.18 | 100 | 200 | 28.0 |
| 2.25 | 70 | 220 | 40.0 |
| 1.919 | 2 | 311 | 47.3 |
| 1.837 | 23 | 222 | 49.6 |
| 1.591 | 10 | 400 | 57.9 |
| 1.460 | <1 | 331 | 63.7 |
| 1.423 | 27 | 420 | 65.5 |
| 1.299 | 19 | 422 | 72.7 |
| 1.225 | <1 | 511 | 77.9 |
| 1.125 | 6 | 440 | 86.4 |
| 1.076 | <1 | 531 | 91.4 |
| 1.061 | 12 | 600 | 93.1 |
| 1.006 | 9 | 620 | 99.9 |
| 0.971 | <1 | 533 | 105.0 |
| .960 | 8 | 622 | 106.8 |
| .919 | 3 | 444 | 113.9 |
| .891 | <1 | 711 | 119.6 |
| .883 | 7 | 640 | 121.5 |
| .851 | 15 | 642 | 129.8 |
| .829 | <1 | 731 | 136.7 |
| .796 | 2 | 800 | 151.0 |

**Structural data.** Picon and Patrie (1956) determined that yttrium sulfide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(YS) per unit cell. The atoms occupy the special positions:

Y: 0 0 0 ;F.C.
S: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

The lattice constant used in this calculated pattern is a = 5.466 Å as reported by Flahaud and Guittard (1956). Iandelli (1961) reports a value a = 5.493 Å.

The calculated density is 4.920 g/cm$^3$, based on the value a = 5.466 Å.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 3.16 | 43 | 111 | 28.2 |
| 2.73 | 100 | 200 | 32.7 |
| 1.933 | 61 | 220 | 47.0 |
| 1.648 | 16 | 311 | 55.7 |
| 1.578 | 19 | 222 | 58.4 |
| 1.366 | 8 | 400 | 68.6 |
| 1.254 | 6 | 331 | 75.8 |
| 1.222 | 21 | 420 | 78.1 |
| 1.116 | 16 | 422 | 87.3 |
| 1.052 | 4 | 511 | 94.2 |
| 0.966 | 6 | 440 | 105.7 |
| .924 | 5 | 531 | 113.0 |
| .911 | 13 | 600 | 115.4 |
| .864 | 10 | 620 | 126.1 |
| .834 | 2 | 533 | 135.0 |
| .824 | 10 | 622 | 138.4 |
| .789 | 4 | 444 | 155.0 |



**Powder diffraction file card.** No. 2-0956, General Electric Co.

**Additional published patterns.** Becker and Ebert (1925) and van Arkel (1924).

**Structural data.** Becker and Ebert (1925) determined that zirconium nitride is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(ZrN) per unit cell. The atoms occupy the special positions:

Zr: 0 0 0 ;F.C.
N: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ ;F.C.

The lattice constant used in this calculated pattern is a = 4.575 Å as reported by Baker (1958).

The calculated density is 7.298 g/cm$^3$.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| d(Å) | I(Peak height) | hkl | 2θ(°) |
|---|---|---|---|
| 2.64 | 100 | 111 | 33.91 |
| 2.29 | 85 | 200 | 39.35 |
| 1.618 | 47 | 220 | 56.87 |
| 1.379 | 32 | 311 | 67.89 |
| 1.321 | 13 | 222 | 71.35 |
| 1.144 | 6 | 400 | 84.67 |
| 1.050 | 13 | 331 | 94.42 |
| 1.023 | 18 | 420 | 97.69 |
| 0.934 | 15 | 422 | 111.1 |
| .880 | 13 | 511 | 122.0 |
| .809 | 8 | 440 | 144.5 |

**Structural data.** Samsonov (1957) determined that zirconium oxide is isostructural with sodium chloride with the space group $O_h^5$-Fm3m (No. 225) and 4(ZrO) per unit cell. The atoms occupy the special positions:

Zr: 0 0 0 ;F.C.
O: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$ ;F.C.

The lattice constant used in this calculated pattern is a = 4.62 Å as reported by Schönberg (1954) The calculated density is 7.22 g/cm$^3$.
Elliott (1965) describes the compound as unstable.

Calculated Pattern
CuK$\alpha_1$ $\lambda$ = 1.5405 Å

| $d$(Å) | $I\left(\frac{Peak}{height}\right)$ | $hkl$ | $2\theta$(°) |
|---|---|---|---|
| 2.67 | 100 | 111 | 33.6 |
| 2.31 | 98 | 200 | 39.0 |
| 1.63 | 55 | 220 | 56.3 |
| 1.39 | 33 | 311 | 67.1 |
| 1.33 | 15 | 222 | 70.6 |
| 1.16 | 7 | 400 | 83.6 |
| 1.06 | 13 | 331 | 93.2 |
| 1.03 | 20 | 420 | 96.4 |
| 0.943 | 17 | 422 | 109.5 |
| .889 | 13 | 511 | 120.1 |
| .817 | 8 | 440 | 141.2 |

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[5] Further work on this program is in progress, and it is anticipated that additional sections will be issued. Therefore, the accumulative index here is not necessarily the concluding index for the project.

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| Gadolinium vanadate, $GdVO_4$ | 5m | 30 |
| Gallium, Ga | 2 | 9 |
| Gallium arsenide, GaAs | 3m | 33 |
| Gallium antimonide, GaSb | 6 | 30 |
| Gallium oxide, alpha, $Ga_2O_3$ | 4 | 25 |
| Gallium phosphate ($\alpha$-quartz type), $GaPO_4$ | 8 | 27 |
| Germanium, Ge | 1 | 18 |
| Germanium dioxide, $GeO_2$ (hexagonal) (low form) | 1 | 51 |
| Germanium dioxide, $GeO_2$ (tetragonal) (high form) | 8 | 28 |
| Germanium iodide, $GeI_2$ | 4m | 58 |
| Germanium(IV) iodide, $GeI_4$ | 5 | 25 |
| Gold, Au | 1 | 33 |
| Gold antimony 1:2 (aurostibite), $AuSb_2$ | 7 | 18 |
| Gold dysprosium, AuDy | 5m | 66 |
| Gold(I) cyanide, AuCN | 10 | 33 |
| Gold holmium, AuHo | 5m | 68 |
| Gold tin, 1:1 AuSn | 7 | 19 |
| Hafnium, Hf | 3 | 18 |
| Holmium arsenate, $HoAsO_4$ | 3m | 34 |
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| Holmium selenide, HoSe | 4m | 59 |
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| Indium antimony, InSb | 4 | 73 |
| Indium arsenide, InAs | 3m | 35 |
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| Indium phosphate, $InPO_4$ | 8 | 29 |
| Iodic acid, $HIO_3$ | 5 | 28 |
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| Lanthanum chloride, $LaCl_3$ | 1m | 20 |
| Lanthanum fluoride, $LaF_3$ | 7 | 21 |
| Lanthanum magnesium, LaMg | 5m | 69 |
| Lanthanum magnesium nitrate 24-hydrate, $La_2Mg_3(NO_3)_{12} \cdot 24H_2O$ | 1m | 22 |
| Lanthanum niobium titanium oxide, $LaNbTiO_6$ | 3m | 37 |
| Lanthanum nitride, LaN | 4m | 61 |
| Lanthanum oxide, $La_2O_3$ | 3 | 33 |
| Lanthanum oxychloride, LaOCl | 7 | 22 |
| Lanthanum phosphide, LaP | 5m | 69 |
| Lanthanum selenide, LaSe | 4m | 61 |
| Lanthanum zinc, LaZn | 5m | 70 |
| Lead, Pb | 1 | 34 |
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| Lead carbonate (cerrussite), $PbCO_3$ | 2 | 56 |


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| Lead fluochloride (matlockite), PbFCl | 1 | 76 |
| Lead fluoride, alpha $PbF_2$ (orthorhombic) | 5 | 31 |
| Lead fluoride, beta $PbF_2$ (cubic) | 5 | 33 |
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| Lead sulfate (anglesite), $PbSO_4$ | 3 | 67 |
| Lead sulfide (galena), PbS | 2 | 18 |
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| Mercury(II) iodide, $HgI_2$ | 1 | 74 |
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| Neodymium chloride, $NdCl_3$ | 1m | 33 |
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| Neodymium fluoride, $NdF_3$ | 8 | 36 |
| Neodymium gallium oxide, $Nd_3Ga_2(GaO_4)_3$ | 1M | 34 |
| Neodymium oxide, $Nd_2O_3$ | 4 | 26 |
| Neodymium oxychloride, NdOCl | 8 | 37 |
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| Praseodymium sulfide, PrS | 4m | 67 |
| Praseodymium vanadate, $PrVO_4$ | 5m | 40 |
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| Samarium fluoride, $SmF_3$ | 1m | 41 |
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| Samarium oxide, $Sm_2O_3$ (cubic) | 4m | 34 |
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| Scandium arsenide, ScAs | 4m | 68 |
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| Strontium boron oxide, $SrB_4O_7$ | 4m | 36 |
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| Strontium molybdate, $SrMoO_4$ | 7 | 50 |
| Strontium nitrate, $Sr(NO_3)_2$ | 1 | 80 |
| Strontium oxide, SrO | 5 | 68 |
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| Strontium sulfate (celestite), $SrSO_4$ | 2 | 61 |
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| Strontium telluride, SrTe | 4m | 69 |
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| Thallium(I) iodide, TlI (orthorhombic) | 4 | 53 |
| Thallium(I) nitrate, $TlNO_3$ | 6 | 58 |
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A mineral name in ( ) indicates a synthetic sample.

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*Natural mineral.

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